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=>
=> d his

     (FILE 'HOME' ENTERED AT 12:07:42 ON 18 JAN 2008)

     FILE 'REGISTRY' ENTERED AT 12:08:03 ON 18 JAN 2008
L1               STRUCTURE UPLOADED
L2            13 S L1 SSS SAM
L3           193 S L1 SSS FULL

     FILE 'HCAPLUS' ENTERED AT 12:09:12 ON 18 JAN 2008
L4            95 S L3
                 E GLUCOSE TRANSPORT+ALL/CT
L5         14191 S (GLUCOSE TRANSPORT OR "GLUCOSE TRANSPORT" OR "BIOLOGICAL TRAN
L6             3 S L5 AND L4

     FILE 'STNGUIDE' ENTERED AT 12:10:02 ON 18 JAN 2008

     FILE 'HCAPLUS' ENTERED AT 12:13:50 ON 18 JAN 2008
L7             2 S SGLI
L8             0 S L7 AND L4

     FILE 'STNGUIDE' ENTERED AT 12:14:30 ON 18 JAN 2008

     FILE 'HCAPLUS' ENTERED AT 12:15:10 ON 18 JAN 2008
L9           253 S SGLT
L10            3 S L9 AND L4
L11            2 S L10 NOT L6

     FILE 'STNGUIDE' ENTERED AT 12:15:50 ON 18 JAN 2008

     FILE 'HCAPLUS' ENTERED AT 12:28:27 ON 18 JAN 2008
L12          611 S FLUOR? GLUC?
L13            0 S L12 AND TRASPORT
L14           70 S L12 AND TRANSPORT
L15           29 S L14 AND METABOLISM
L16            0 S L15 AND L4
L17            1 S L14 AND L4
L18           27 S L15 AND 1800<=PY<=2003

     FILE 'STNGUIDE' ENTERED AT 12:31:42 ON 18 JAN 2008

     FILE 'STNGUIDE' ENTERED AT 12:44:36 ON 18 JAN 2008

     FILE 'HCAPLUS' ENTERED AT 12:44:53 ON 18 JAN 2008
L19            2 S L4 AND DRUG

     FILE 'STNGUIDE' ENTERED AT 12:45:18 ON 18 JAN 2008

     FILE 'HCAPLUS' ENTERED AT 12:46:28 ON 18 JAN 2008

     FILE 'STNGUIDE' ENTERED AT 12:46:28 ON 18 JAN 2008

     FILE 'STNGUIDE' ENTERED AT 12:46:33 ON 18 JAN 2008

     FILE 'STNGUIDE' ENTERED AT 13:03:50 ON 18 JAN 2008

=> fil hcaplus
COST IN U.S. DOLLARS                        SINCE FILE      TOTAL
                                              ENTRY    SESSION
FULL ESTIMATED COST                             1.32     335.99

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)  SINCE FILE      TOTAL
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                                                    ENTRY    SESSION
CA SUBSCRIBER PRICE                                  0.00     -25.60

FILE 'HCAPLUS' ENTERED AT 13:16:47 ON 18 JAN 2008
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FILE COVERS 1907 - 18 Jan 2008  VOL 148 ISS 4
FILE LAST UPDATED: 17 Jan 2008  (20080117/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> s l4 not l6
L20          92 L4 NOT L6

=> s l20 not l11
L21          90 L20 NOT L11

=> s l21 not l18
L22          90 L21 NOT L18

=> s l22 not l17
L23          90 L22 NOT L17

=> S L23 AND 1800<=PY<=2003
      23975279 1800<=PY<=2003
L24          80 L23 AND 1800<=PY<=2003

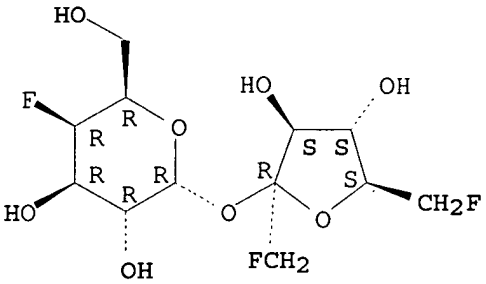
=> s l24 and (diabetes OR "Diabetes" OR "Diabetes insipidus" OR "Diabetes mellitus")
         135781 DIABETES
         135781 "DIABETES"
         135781 "DIABETES"
           3751 "INSIPIDUS"
           3740 "DIABETES INSIPIDUS"
                  ("DIABETES"(W)"INSIPIDUS")
         135781 "DIABETES"
         100164 "MELLITUS"
         100096 "DIABETES MELLITUS"
                  ("DIABETES"(W)"MELLITUS")
L25           0 L24 AND (DIABETES OR "DIABETES" OR "DIABETES INSIPIDUS" OR "DIAB
                ETES MELLITUS")

=> d l24 ibib abs hitstr 1-10

L24  ANSWER 1 OF 80  HCAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2004:861485  HCAPLUS
DOCUMENT NUMBER:          143:131949
TITLE:                    Study on relationship between structure and sweetness
```

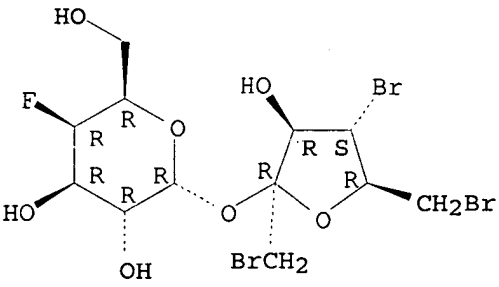
of sucrose derivatives
AUTHOR(S): Zheng, Jianxian; Rao, Zhijuan; Jia, Chengxiang
CORPORATE SOURCE: College of Food and Bio-engineering, Huanan University of Science and Technology, Guangzhou, 510640, Peop. Rep. China
SOURCE: Shipin Kexue (Beijing, China) (2003), 24(5), 29-33
CODEN: SPKHD5; ISSN: 1002-6630
PUBLISHER: Zhongguo Shipin Zazhishe
DOCUMENT TYPE: Journal; General Review
LANGUAGE: Chinese
AB A review with 15 reference was given on the relationship between structure and sweetness of sucrose derivs. The sweetness mechanism of sucrose derivs. was essentially explained by the AHB-γ theory and the multipoint attachment theory.
IT 475491-24-8 591229-87-7
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(structure and sweetness of sucrose derivs.)
RN 475491-24-8 HCAPLUS
CN α-D-Galactopyranoside, 1,6-dideoxy-1,6-difluoro-β-D-fructofuranosyl 4-deoxy-4-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 591229-87-7 HCAPLUS
CN α-D-Galactopyranoside, (2R,3R,4S,5R)-4-bromo-2,5-bis(bromomethyl)tetrahydro-3-hydroxy-2-furanyl 4-deoxy-4-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

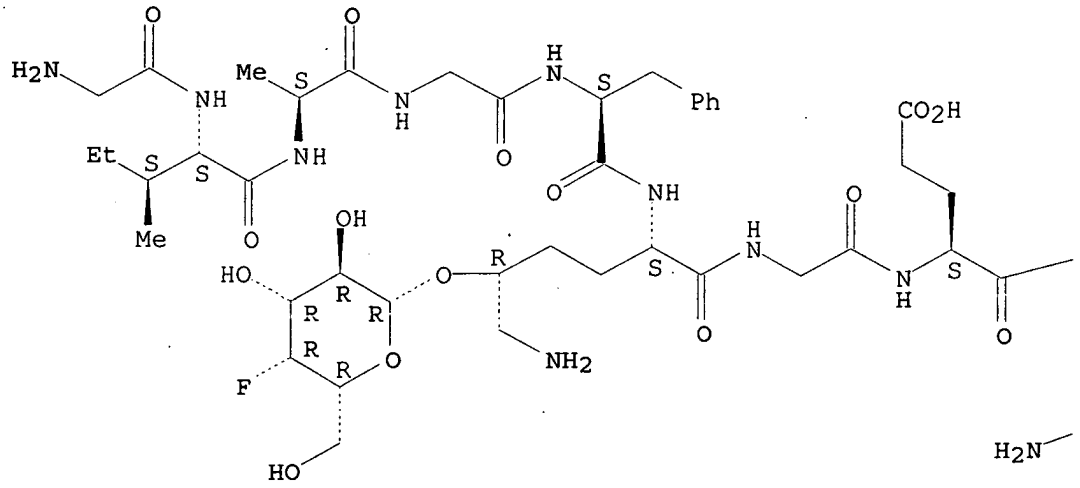


L24 ANSWER 2 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:645692 HCAPLUS
DOCUMENT NUMBER: 139:379830
TITLE: Role of the galactosyl moiety of collagen glycopeptides for T-cell stimulation in a model for rheumatoid arthritis
AUTHOR(S): Holm, Bjorn; Baquer, Syed M.; Holm, Lotta; Holmdahl,

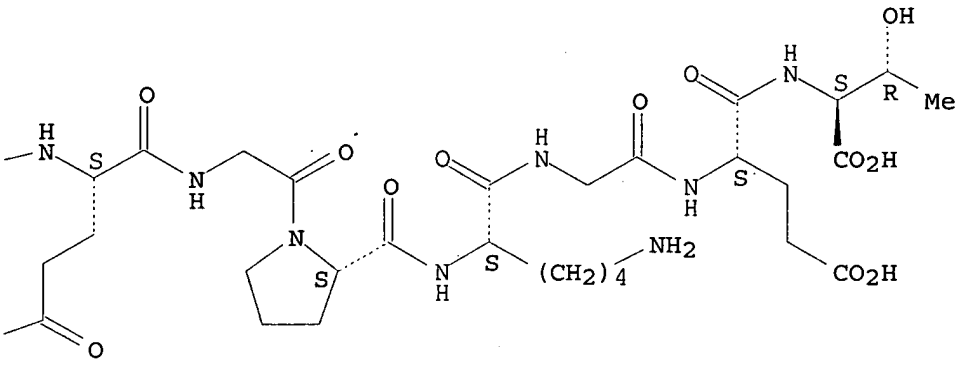
Rikard; Kihlberg, Jan
CORPORATE SOURCE: Department of Chemistry, Organic Chemistry, Umea University, Umea, SE-901 87, Swed.
SOURCE: Bioorganic & Medicinal Chemistry (2003), 11(18), 3981-3987
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Two protected derivs. of β-D-galactopyranosyl-5-hydroxy-L-lysine, in which HO-4 of galactose has been O-methylated or replaced by fluorine, have been prepared The building blocks were incorporated at position 264 of the peptide fragment CII259-273 from type II collagen by solid-phase synthesis. The ability of these two glycopeptides, and two CII259-273 glycopeptides in which HO-4 of galactose was either unmodified or deoxygenated, to elicit responses from T-cell hybridomas obtained in a mouse model for rheumatoid arthritis was then determined The hybridomas were all highly sensitive towards modifications at C-4 of the β-d-galactosyl residue of CII259-273, highlighting the role of HO-4 as an important contact point for the T-cell receptor. Most likely, this glycopeptide hydroxyl group is involved in hydrogen bonding with the T-cell receptor.
IT 623574-50-5P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(in preparation of galactose-containing glycopeptides from collagen for study of glycopeptide recognition by T-cells in rheumatoid arthritis)
RN 623574-50-5 HCAPLUS
CN L-Threonine, glycyl-L-isoleucyl-L-alanylglycyl-L-phenylalanyl-(5R)-5-[(4-deoxy-4-fluoro-β-D-galactopyranosyl)oxy]-L-lysylglycyl-L-α-glutamyl-L-glutaminylglycyl-L-prolyl-L-lysylglycyl-L-α-glutamyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



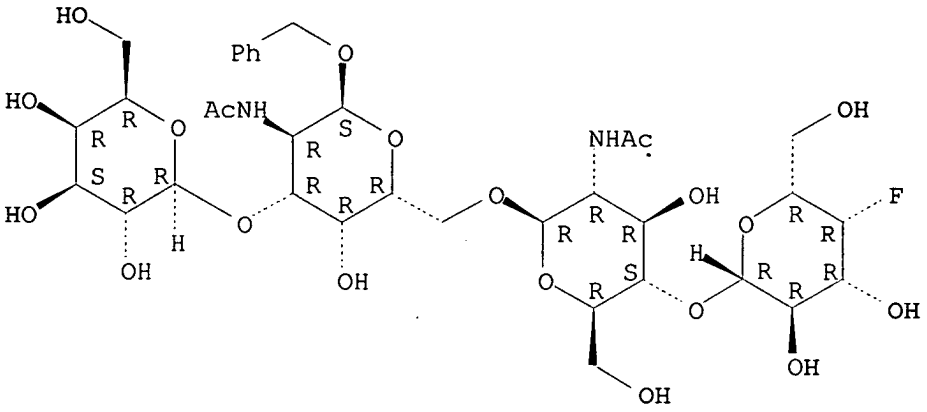
PAGE 1-B



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 3 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:590199 HCAPLUS
DOCUMENT NUMBER: 140:42384
TITLE: Synthesis of fluorine-containing core-2 tetrasaccharides
AUTHOR(S): Xia, Jie; Alderfer, James L.; Piskorz, Conrad F.; Locke, Robert D.; Matta, Khushi L.
CORPORATE SOURCE: Molecular and Cellular Biophysics, Roswell Park Cancer Institute, Buffalo, NY, 14263, USA
SOURCE: Synlett (2003), (9), 1291-1294
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:42384
AB Synthesis of core-2 branched tetrasaccharides, in which a fluorine atom was substituted at the 3 or 4-position of galactose residues is described.
IT 635301-71-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of fluorine-containing core-2 branched tetrasaccharides where the fluorine atom is at the 3- or 4-position of the galactose residues)
RN 635301-71-2 HCAPLUS
CN α-D-Galactopyranoside, phenylmethyl O-4-deoxy-4-fluoro-β-D-galactopyranosyl-(1→4)-O-2-(acetylamino)-2-deoxy-β-D-glucopyranosyl-(1→6)-O-[β-D-galactopyranosyl-(1→3)]-2-(acetylamino)-2-deoxy- (CA INDEX NAME)

Absolute stereochemistry.



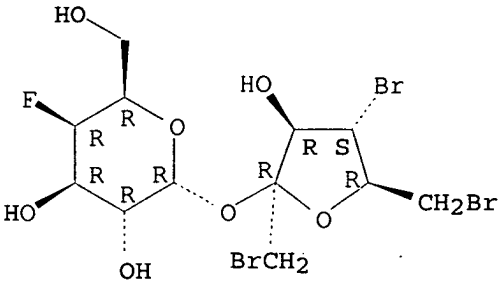
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 4 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:453562 HCAPLUS
DOCUMENT NUMBER: 139:230903
TITLE: Synthesis and taste properties of 4,1',4',6'-tetrahalodeoxysucrose analogues
AUTHOR(S): Sofian, A. S. Md; Lee, C. Kuan
CORPORATE SOURCE: Department of Chemistry, National University of Singapore, Singapore, 119260, Singapore
SOURCE: Journal of Carbohydrate Chemistry (2003), 22(3 & 4), 185-206
CODEN: JCACDM; ISSN: 0732-8303
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:230903

AB The synthesis of a series of 1,4,6-trideoxy-1,4,6-trihalo-β-D-hexulofuranosyl 4-deoxy-4-halo-β-D-hexopyranosides is described. The 4-chloro-, 4-bromo- and 4-iodo-4-deoxy-β-D-fructofuranosyl analogs were synthesized from a 3',4'-lyxo-epoxide using the resp. alkali metal halides. The corresponding 4-halodeoxytagatofuranosyl analogs, on the other hand, were obtained by direct halide displacement of the 4'-O-trifluoromethanesulfonyl derivative, which was derived by regioselective sulfonylation of 1,6-di-O-trityl-β-D-fructofuranosyl 6-O-trityl-α-D-glucopyranoside via its stannylene acetal. The sweetness intensities of these tetrahalodeoxy compds. strongly suggest that both size and configuration of the halogen substituents at C-4 and C-4' are critical for sweetness enhancement.

IT 591229-87-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(synthesis and taste properties of tetrahalodeoxysucrose analogs)
RN 591229-87-7 HCAPLUS
CN α-D-Galactopyranoside, (2R,3R,4S,5R)-4-bromo-2,5-bis(bromomethyl)tetrahydro-3-hydroxy-2-furanyl 4-deoxy-4-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

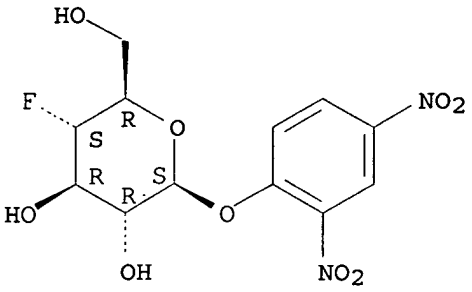
L24 ANSWER 5 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:860324 HCAPLUS
DOCUMENT NUMBER: 138:38897
TITLE: Equatorial Contra Axial Polar Substituents. The Relation of a Chemical Reaction to Stereochemical Substituent Constants
AUTHOR(S): Bols, Mikael; Liang, Xifu; Jensen, Henrik H.
CORPORATE SOURCE: Department of Chemistry, Aarhus University, Aarhus, DK-8000, Den.
SOURCE: Journal of Organic Chemistry (2002), 67(25), 8970-8974
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:38897

AB The established rates of glycoside hydrolysis reactions were analyzed using free energy relation plots based on substituent consts. that depend on whether the substituent is axial or equatorial. In all cases good correlations were found when assuming either that the transition state had a charged ring-O atom or that it had a charged anomeric C atom. The spontaneous hydrolysis of 2,4-dinitrophenyl β-glycopyranosides and the acidic hydrolysis of Me β-D-glycopyranosides gave a good correlation, when 100% charge at the ring-O in the transition state of these reactions is assumed. The acidic hydrolysis of Me α-glycopyranosides gave good correlations regardless of whether 100% charge at the ring-O or 100% charge at the anomeric C was assumed. Crucial the stereochem. of even remote polar substituents is for their electronic effect on chemical reaction.

IT 171626-62-3
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(reinterpretation of hydrolysis kinetics; equatorial vs. axial polar substituents and relation of chemical reaction to stereochem. substituent consts.)

RN 171626-62-3 HCAPLUS
CN β-D-Glucopyranoside, 2,4-dinitrophenyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



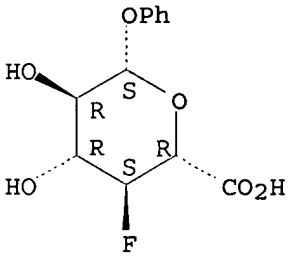
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 6 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:690164 HCAPLUS
DOCUMENT NUMBER: 138:119155
TITLE: Development of an assay and determination of kinetic parameters for chondroitin AC lyase using defined synthetic substrates
AUTHOR(S): Rye, Carl S.; Withers, Stephen G.
CORPORATE SOURCE: Department of Chemistry, University of British Columbia, Vancouver, BC, V6T 1Z1, Can.
SOURCE: Analytical Biochemistry (2002), 308(1), 77-82
CODEN: ANBCA2; ISSN: 0003-2697
PUBLISHER: Elsevier Science
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Many techniques have been developed for the assay of polysaccharide lyases; however, due to the inhomogeneous nature of the polymeric substrates none have allowed the measurement of defined and reproducible kcat and Km values. We have designed three different substrates for chondroitin AC lyase from Flavobacterium heparinum that can be monitored by three different techniques: UV/Vis spectroscopy, fluorescence spectroscopy, and use of a fluoride ion-selective electrode. Each is a continuous assay, free from interferences caused by other components present in crude enzyme prepns., and allows meaningful and reproducible kinetic parameters to be determined The development of these defined synthetic substrates has opened up a wide variety of mechanistic studies that can be performed to elucidate the detailed catalytic mechanism of this and other polysaccharide lyases. The application of these techniques, which include kinetic isotope effects and linear free energy analyses, was not possible with the previous polymeric substrates and will allow this relatively poorly understood class of polysaccharide-degrading enzymes to be studied mechanistically.

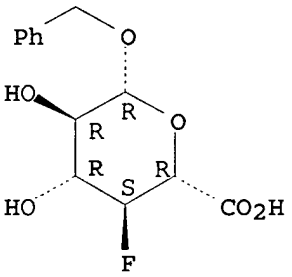
IT 461025-88-7 461025-89-8
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(synthetic substrates permit assay of chondroitin AC lyase by UV/Vis spectroscopy, fluorescence spectroscopy, and fluoride ion-selective electrode)
RN 461025-88-7 HCAPLUS
CN β-D-Glucopyranosiduronic acid, phenyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



RN 461025-89-8 HCAPLUS
CN β-D-Glucopyranosiduronic acid, phenylmethyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 7 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:640072 HCAPLUS
DOCUMENT NUMBER: 137:365286
TITLE: Computational studies of sweet-tasting molecules
AUTHOR(S): Barker, Jodie S.; Hattotuwagama, Channa K.; Drew, Michael G. B.
CORPORATE SOURCE: Department of Chemistry, University of Reading, Reading, RG6 6AD, UK
SOURCE: Pure and Applied Chemistry (2002), 74(7), 1207-1217
CODEN: PACHAS; ISSN: 0033-4545
PUBLISHER: International Union of Pure and Applied Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Quant. structure-activity relationships (QSARs) are developed for two sep. families of sweet-tasting mols. for which sweetness values relative to sucrose (RS) have been measured. For these two families of sucrose and guanidine derivs., the mols. were divided into training and test sets. Linear multiple regression equations have been generated to relate sep. log(RS) to two types of parameters, namely mol. descriptors and energies derived via mol. field anal. (MFA). The parameters used in the development of linear multiple regression equations were selected by the genetic algorithm. The equations obtained show high predictive quality, which is confirmed by statistical parameters obtained with the test sets. The data for these two families were then combined with data from two other families previously studied, namely the sulfamates and isovanillates, to make a set of 149 compds. These mols. were also studied by QSAR methods. The generated equations show remarkable predictive power, and the quality of the results suggest that the mechanism of sweet taste receptor is similar and, therefore, that there could well be only one receptor site for sweet taste, particularly for the four sweet taste

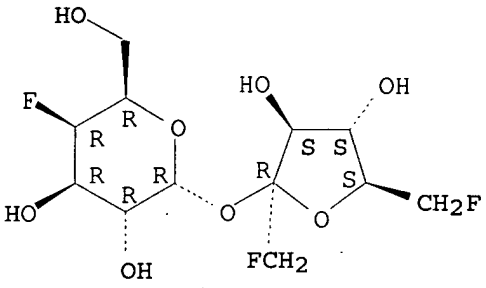
families considered in this work.

IT 475491-24-8
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(computational studies of sweet-tasting mols.)

RN 475491-24-8 HCAPLUS

CN α-D-Galactopyranoside, 1,6-dideoxy-1,6-difluoro-β-D-fructofuranosyl 4-deoxy-4-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 8 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:552597 HCAPLUS
DOCUMENT NUMBER: 137:243862
TITLE: Elucidation of the Mechanism of Polysaccharide Cleavage by Chondroitin AC Lyase from Flavobacterium heparinum
AUTHOR(S): Rye, Carl S.; Withers, Stephen G.
CORPORATE SOURCE: Department of Chemistry, University of British Columbia, Vancouver, BC, V6T 1Z1, Can.
SOURCE: Journal of the American Chemical Society (2002), 124(33), 9756-9767
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:243862

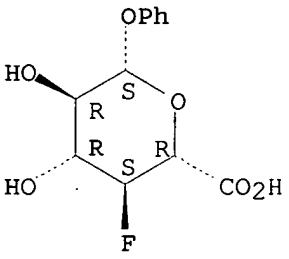
AB Chondroitin AC lyase from Flavobacterium heparinum degrades chondroitin sulfate glycosaminoglycans via an elimination mechanism resulting in disaccharides or oligosaccharides with Δ4,5-unsatd. uronic acid residues at their nonreducing end. Mechanistic details concerning the ordering of the bond-breaking and -forming steps of this enzymic reaction are nonexistent, mainly due to the inhomogeneous nature of the polymeric substrates. The creation of a new class of synthetic substrates for this enzyme has allowed the measurement of defined and reproducible kcat and Km values and has expanded the range of mechanistic studies that can be performed. The primary deuterium kinetic isotope effect upon kcat/Km for the abstraction of the proton α to the carboxylic acid was measured to be 1.67±0.07, showing that deprotonation occurs in a rate-limiting step. Using substrates with leaving groups of differing reactivity, a flat linear free energy relationship was produced, indicating that the C4-O4 bond is not broken in a rate-determining step. Taken together, these results strongly suggest a stepwise mechanism. Consistent with this was the measurement of a secondary deuterium kinetic isotope effect upon kcat/Km of 1.01±0.03 on a 4-{2H}-substrate, indicating that no sp2 character is developed at C4 during the rate-limiting step, thereby ruling out a concerted syn-elimination.

IT 461025-88-7P 461026-01-7P

RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(elucidation of mechanism of polysaccharide cleavage by chondroitin AC lyase from Flavobacterium heparinum and synthesis of substrates)

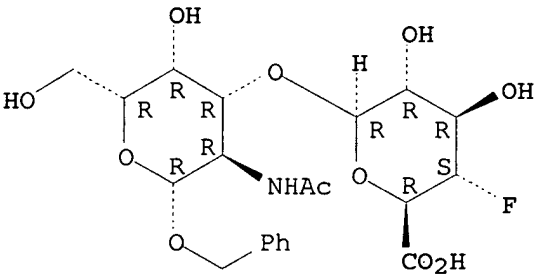
RN 461025-88-7 HCAPLUS
CN β-D-Glucopyranosiduronic acid, phenyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



RN 461026-01-7 HCAPLUS
CN β-D-Galactopyranoside, phenylmethyl 2-(acetylamino)-2-deoxy-3-O-(4-deoxy-4-fluoro-β-D-glucopyranuronosyl)- (CA INDEX NAME)

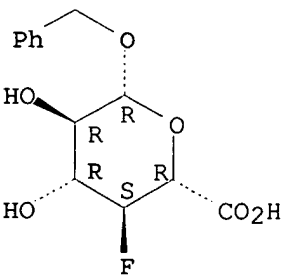
Absolute stereochemistry.



IT 461025-89-8P 461025-90-1P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(elucidation of mechanism of polysaccharide cleavage by chondroitin AC lyase from Flavobacterium heparinum and synthesis of substrates)

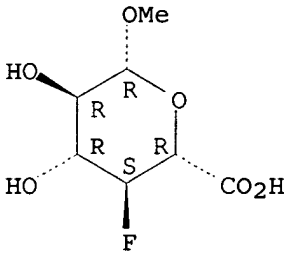
RN 461025-89-8 HCAPLUS
CN β-D-Glucopyranosiduronic acid, phenylmethyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



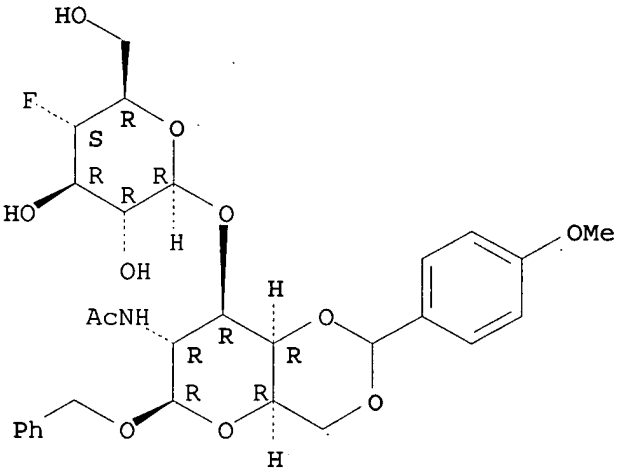
RN 461025-90-1 HCAPLUS
CN β-D-Glucopyranosiduronic acid, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



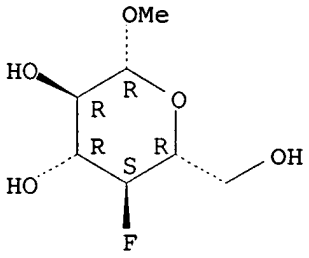
IT 461026-43-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(elucidation of mechanism of polysaccharide cleavage by chondroitin AC lyase from Flavobacterium heparinum and synthesis of substrates)
RN 461026-43-7 HCAPLUS
CN β-D-Galactopyranoside, phenylmethyl 2-(acetylamino)-2-deoxy-3-O-(4-deoxy-4-fluoro-β-D-glucopyranosyl)-4,6-O-[(4-methoxyphenyl)methylene]- (CA INDEX NAME)

Absolute stereochemistry.



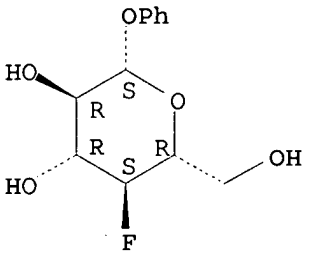
IT 141990-24-1P 461025-83-2P 461025-85-4P
461026-00-6P 461026-05-1P 461026-41-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(elucidation of mechanism of polysaccharide cleavage by chondroitin AC lyase from Flavobacterium heparinum and synthesis of substrates)
RN 141990-24-1 HCAPLUS
CN β-D-Glucopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



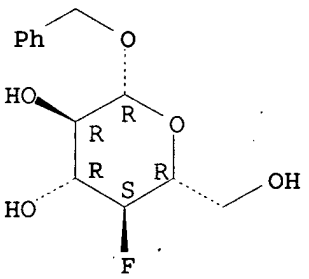
RN 461025-83-2 HCAPLUS
CN β-D-Glucopyranoside, phenyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



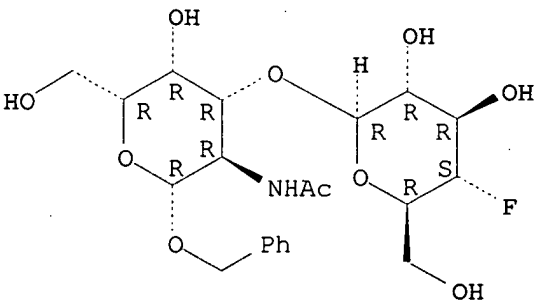
RN 461025-85-4 HCAPLUS
CN β-D-Glucopyranoside, phenylmethyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



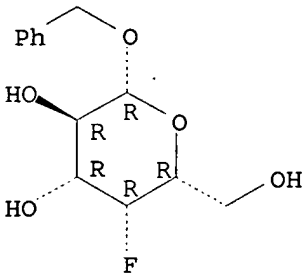
RN 461026-00-6 HCAPLUS
CN β-D-Galactopyranoside, phenylmethyl 2-(acetylamino)-2-deoxy-3-O-(4-deoxy-4-fluoro-β-D-glucopyranosyl)- (CA INDEX NAME)

Absolute stereochemistry.



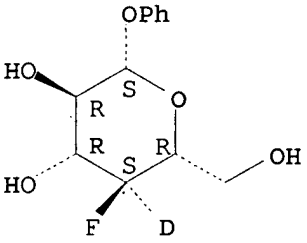
RN 461026-05-1 HCAPLUS
CN β-D-Galactopyranoside, phenylmethyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



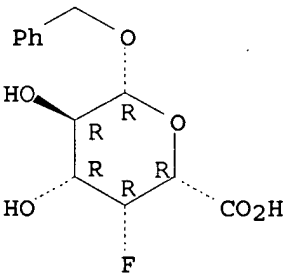
RN 461026-41-5 HCAPLUS
CN β-D-xylo-Hexopyranoside-4-d, phenyl 4-deoxy-4-fluoro-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



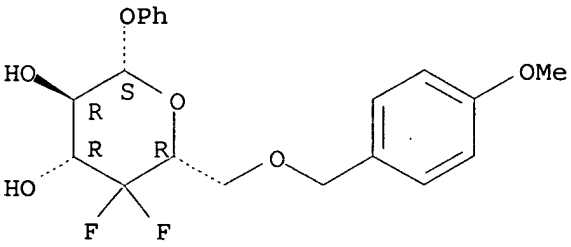
IT 461026-06-2P 461026-12-0P 461026-38-0P
461026-42-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(elucidation of mechanism of polysaccharide cleavage by chondroitin AC lyase from Flavobacterium heparinum and synthesis of substrates)
RN 461026-06-2 HCAPLUS
CN β-D-Galactopyranosiduronic acid, phenylmethyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



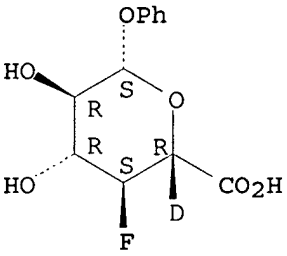
RN 461026-12-0 HCAPLUS
CN β-D-xylo-Hexopyranoside, phenyl 4-deoxy-4,4-difluoro-6-O-[(4-methoxyphenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.



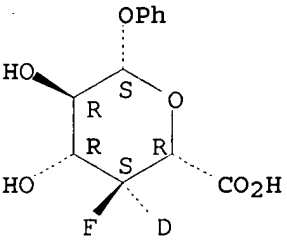
RN 461026-38-0 HCAPLUS
CN β-D-Glucopyranosiduronic-5-C-d acid, phenyl 4-deoxy-4-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 461026-42-6 HCAPLUS
CN β-D-xylo-Hexopyranosiduronic-4-d acid, phenyl 4-deoxy-4-fluoro-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 68 THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 9 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:466160 HCAPLUS
DOCUMENT NUMBER: 137:43451
TITLE: Crystal structure of the ligand-binding site of Neisseria meningitidis LgtC galactosyltransferase and other retaining glycosyltransferases and application to drug discovery
INVENTOR(S): Withers, Stephen G.; Wakarchuk, Warren W.; Strynadka, Natalie C. J.; Dieckelmann, Manuela; Ly, Hoa; Persson, Karina
PATENT ASSIGNEE(S): The University of British Columbia, Can.
SOURCE: PCT Int. Appl., 204 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

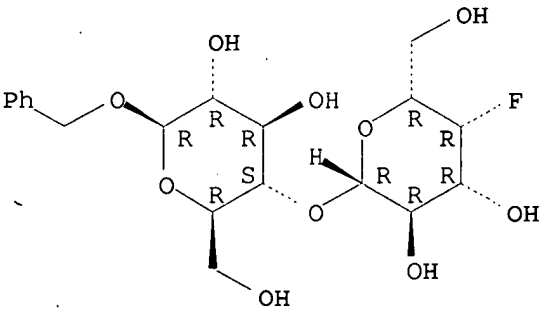
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002048320	A2	20020620	WO 2001-CA1793	20011214 <--
WO 2002048320	A3	20021212		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2431901	A1	20020620	CA 2001-2431901	20011214 <--
AU 2002015769	A5	20020624	AU 2002-15769	20011214 <--
US 2004096951	A1	20040520	US 2003-450802	20031117
PRIORITY APPLN. INFO.:			US 2000-255636P P	20001214
			WO 2001-CA1793 W	20011214

AB The present invention relates to a crystal comprising the ligand-binding pocket of a glycosyltransferase and optionally a donor mol. or analog thereof and/or an acceptor mol. or analog thereof. The three-dimensional structure of the retaining gene lgtC galactosyltransferase from Neisseria meningitidis in complex with manganese and substrate analogs (UDP 2-deoxy-2-fluoro-galactose, 4-deoxylactose and lactose) is disclosed. Synthesis of alternate acceptor substrates and inhibitors of the LgtC galactosyltransferase is described. Determination of this first three-dimensional structure of a retaining nucleotide sugar-dependent glycosyltransferase in a complex with analogs of both substrates for the enzyme provides unique insights into the structure and mechanism of this important class of enzymes. The present invention also relates to the use of such a crystal to identify ligands capable of modulating glycosyltransferase activity, and the use of such ligands in therapeutic applications.

IT 431881-82-2P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis of alternate acceptor substrates and inhibitors; crystal structure of ligand-binding site of Neisseria meningitidis LgtC galactosyltransferase and other retaining glycosyltransferases and application to drug discovery)

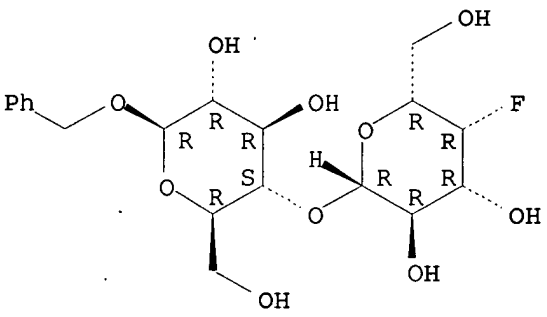
RN 431881-82-2 HCAPLUS
CN β-D-Glucopyranoside, phenylmethyl 4-O-(4-deoxy-4-fluoro-β-D-galactopyranosyl)- (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 10 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:312576 HCAPLUS
DOCUMENT NUMBER: 139:113558
TITLE: Mechanistic studies of a retaining α-galactosyltransferase from Neisseria meningitidis, [Erratum to document cited in CA137:2344]
AUTHOR(S): Ly, Hoa D.; Lougheed, Brenda; Wakarchuk, Warren W.; Withers, Stephen G.
CORPORATE SOURCE: Department of Chemistry, University of British Columbia, Vancouver, BC, V6T 1Z1, Can.
SOURCE: Biochemistry (2002), 41(20), 6572
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB On page 5084, the Note Added in Proof should have appeared as follows: "A recent determination of the structure of the bovine galactosyltransferase (43) casts serious doubts upon the conclusions of the paper by Gastinel et al. (15) concerning the formation of a covalent intermediate.".
IT 431881-82-2P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(retaining lipopolysaccharyl α-galactosyltransferase from Neisseria meningitidis exhibits ordered bi-bi kinetic mechanism (Erratum))
RN 431881-82-2 HCAPLUS
CN β-D-Glucopyranoside, phenylmethyl 4-O-(4-deoxy-4-fluoro-β-D-galactopyranosyl)- (CA INDEX NAME)

Absolute stereochemistry.



=> fil stng

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	62.57	398.56

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-8.00	-33.60

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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jan 11, 2008 (20080111/UP).

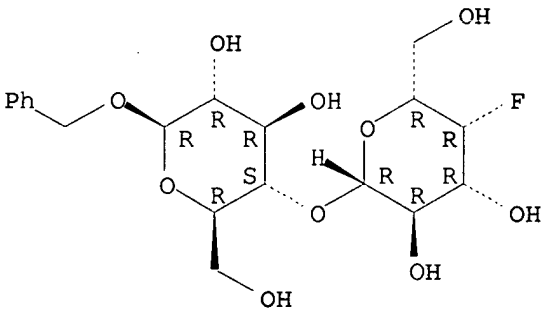
=> d l24 ibib abs hitstr 11-20
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:y

L24 ANSWER 11 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:229529 HCAPLUS
DOCUMENT NUMBER: 137:2344
TITLE: Mechanistic Studies of a Retaining α-Galactosyltransferase from Neisseria meningitidis
AUTHOR(S): Ly, Hoa D.; Lougheed, Brenda; Wakarchuk, Warren W.; Withers, Stephen G.
CORPORATE SOURCE: Department of Chemistry, University of British Columbia, Vancouver, BC, V6T 1Z1, Can.
SOURCE: Biochemistry (2002), 41(16), 5075-5085
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:2344

AB Lipopolysaccharyl α-galactosyltransferase from Neisseria meningitidis catalyzes the transfer of a galactosyl moiety from the activated donor UDP-Gal to glycoconjugates to yield an elongated saccharide product with net retention of anomeric configuration relative to the donor substrate. Through kinetic analyses in which the concns. of both substrates are independently varied and through inhibition studies with dead-end analogs of both substrates and with the oligosaccharide product, we have demonstrated that this enzyme follows an ordered bi-bi kinetic mechanism. Various aspects of the chemical mechanism including the possible formation of a covalent glycosyl-enzyme intermediate were also probed using an assortment of strategies. While the results of these investigations were unable to clearly delineate the chemical mechanism of this enzyme, they provide important insights into the catalytic machinery surrounding the events involved in catalysis.

IT 431881-82-2P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(retaining lipopolysaccharyl α-galactosyltransferase from Neisseria meningitidis exhibits ordered bi-bi kinetic mechanism)
RN 431881-82-2 HCAPLUS
CN β-D-Glucopyranoside, phenylmethyl 4-O-(4-deoxy-4-fluoro-β-D-galactopyranosyl)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 12 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:826100 HCAPLUS
DOCUMENT NUMBER: 136:110274
TITLE: Two halodeoxy sucrose analogues
AUTHOR(S): Linden, Anthony; Lee, C. Kuan; Muhammad Sofian, A. S.
CORPORATE SOURCE: Institute of Organic Chemistry, University of Zuerich, Zurich, CH-8057, Switz.
SOURCE: Acta Crystallographica, Section C: Crystal Structure Communications (2001), C57(11), 1363-1366
CODEN: ACSCEE; ISSN: 0108-2701
PUBLISHER: Munksgaard International Publishers Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

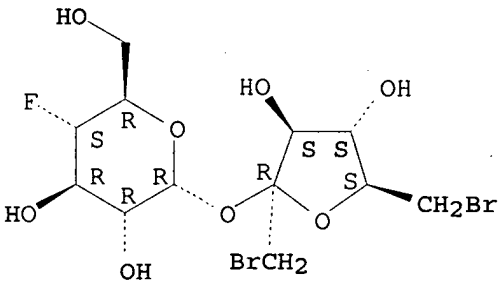
AB At 160 K, the structure of 4-bromo-4-deoxysucrose, C12H21BrO10, is very similar to that of sucrose, particularly with respect to the conformation of the glycosidic linkage. As in sucrose, an intramol. H bond exists between the glucopyranosyl and the fructofuranosyl rings. Conversely, the structure of 1',6'-dibromo-4-fluoro-4,1',6'-trideoxysucrose monohydrate, C12H19Br2FO8·H2O, shows large conformational differences when compared with the structures of both sucrose and sucralose. This compound does not exhibit any intramol. H bonds. In each compound, a complex series of intermol. H bonds link the mols. into an infinite three-dimensional framework. The absolute configuration of each mol. was determined Crystallog. data are given.

IT 389608-28-0P, 1',6'-Dibromo-4-fluoro-4,1',6'-trideoxysucrose monohydrate
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)

RN 389608-28-0 HCAPLUS

CN α-D-Glucopyranoside, 1,6-dibromo-1,6-dideoxy-β-D-fructofuranosyl 4-deoxy-4-fluoro-, monohydrate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● H_2O

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 13 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:76611 HCAPLUS
DOCUMENT NUMBER: 132:251305
TITLE: The Role of Sugar Substituents in Glycoside Hydrolysis
AUTHOR(S): Namchuk, Mark N.; McCarter, John D.; Becalski, Adam; Andrews, Trevor; Withers, Stephen G.
CORPORATE SOURCE: Department of Chemistry, University of British Columbia, Vancouver, BC, V6T 1Z1, Can.
SOURCE: Journal of the American Chemical Society (2000), 122(7), 1270-1277

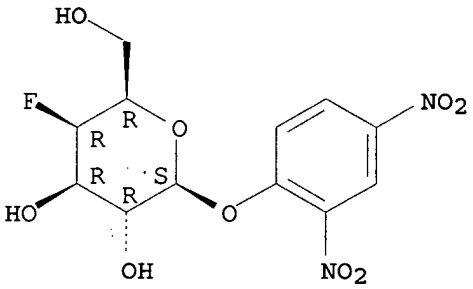
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of monosubstituted deoxy and deoxyfluoro 2,4-dinitrophenyl (DNP) β-D-glycopyranosides was synthesized and used to probe the mechanism of spontaneous β-glycoside hydrolysis. Their relative rates of hydrolysis followed the order 2-deoxy > 4-deoxy > 3-deoxy ≈ 6-deoxy > parent > 6-deoxy-6-fluoro > 3-deoxy-3-fluoro > 4-deoxy-4-fluoro > 2-deoxy-2-fluoro. Hammett correlations of the pH-independent hydrolysis rates of each of the 6-, 4-, 3-, and 2-position substituted glycosides with the σI value for the sugar ring substituent were linear (r = 0.95 to 0.999, ρI = -2.2 to -10.7), consistent with hydrolysis rates being largely dictated by field effects on an electron-deficient transition state. The relative rates of hydrolysis of the DNP glucosides can be rationalized on the basis of the stabilities of the oxocarbenium ion-like transition states, as predicted by the Kirkwood-Westheimer model. The primary determinant of the rate of hydrolysis within a series appears to be the field effect of the ring substituent on O5, the principal center of charge development at the transition state. Differences in the rates of hydrolysis between different series of hexopyranosides may not arise solely from field effects and likely also reflect differences in steric factors or solvation.

IT 144220-98-4P 171626-62-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(role of sugar substituents in glycoside hydrolysis)

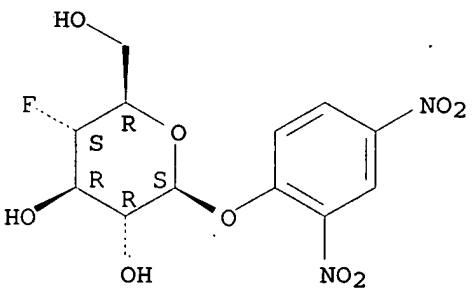
RN 144220-98-4 HCAPLUS
CN β-D-Galactopyranoside, 2,4-dinitrophenyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



RN 171626-62-3 HCAPLUS
CN β-D-Glucopyranoside, 2,4-dinitrophenyl 4-deoxy-4-fluoro- (CA INDEX NAME)

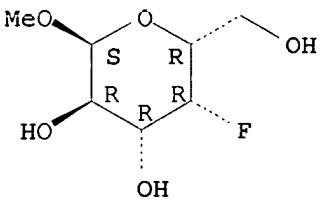
Absolute stereochemistry.



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 14 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:569666 HCAPLUS
DOCUMENT NUMBER: 129:288908
TITLE: Binding of modified fragments of the Shigella dysenteriae type 1 O-specific polysaccharide to monoclonal IgM 3707 E9 and docking of the immunodeterminant to its modeled Fv
AUTHOR(S): Miller, Charles E.; Mulard, Laurence A.; Padlan, Eduardo A.; Glaudemans, Cornelis P. J.
CORPORATE SOURCE: National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health, Bethesda, MD, 20892, USA
SOURCE: Carbohydrate Research (1998), 309(3), 219-226
CODEN: CRBRAT; ISSN: 0008-6215
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The O-specific polysaccharide (O-SP) of Shigella dysenteriae type 1 has been shown by others to have the structure →3)-α-L-Rhap-(1→3)-α-L-Rhap-(1→2)-α-D-Galp-(1→3)-α-D-GlcpNAc-(1→. The authors have shown in the past that IgM 3707 E9, an anti S. dysenteriae type 1 O-SP monoclonal antibody, binds specifically to the -α-L-Rhap-(1→2)-α-D-Galp- determinant of the polysaccharide. In this report the authors show that determinant to have hydrogen bonds, necessary for binding to the antibody, involving positions 3, 4 and 6 of the galactopyranosyl residue. The hydroxyl groups of the rhamnopyranosyl moiety of the immunodeterminant appear not to partake in hydrogen-bond interactions with the antibody. A model is presented of the Fv of IgM 3707 E9 based on the previously established cDNA-sequence and two known, highly homologous Ig crystal structures. The Me glycoside of the immunodeterminant α-L-rhamnopyranosyl-(1→2)-α-D-galactopyranose is docked to the combining area of the Fv.
IT 32934-07-9
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(binding of Shigella dysenteriae O-specific immunodeterminant and related ligands to monoclonal IgM and docking of determinant to Fv fragment)
RN 32934-07-9 HCAPLUS
CN α-D-Galactopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 15 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:639909 HCAPLUS
DOCUMENT NUMBER: 127:314520

TITLE: Biochemical characterization of glycyrrhizin as an effective inhibitor for hyaluronidases from bovine testis

AUTHOR(S): Furuya, Teisuke; Yamagata, Shigeharu; Shimoyama, Yoshihito; Fujihara, Michio; Morishima, Naohiko; Ohtsuki, Kenzo

CORPORATE SOURCE: Laboratory of Genetical Biochemistry, School of Allied Health Sciences, Kitasato University, Sagamihara, 228, Japan

SOURCE: Biological & Pharmaceutical Bulletin (1997), 20(9), 973-977
CODEN: BPBLEO; ISSN: 0918-6158

PUBLISHER: Pharmaceutical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

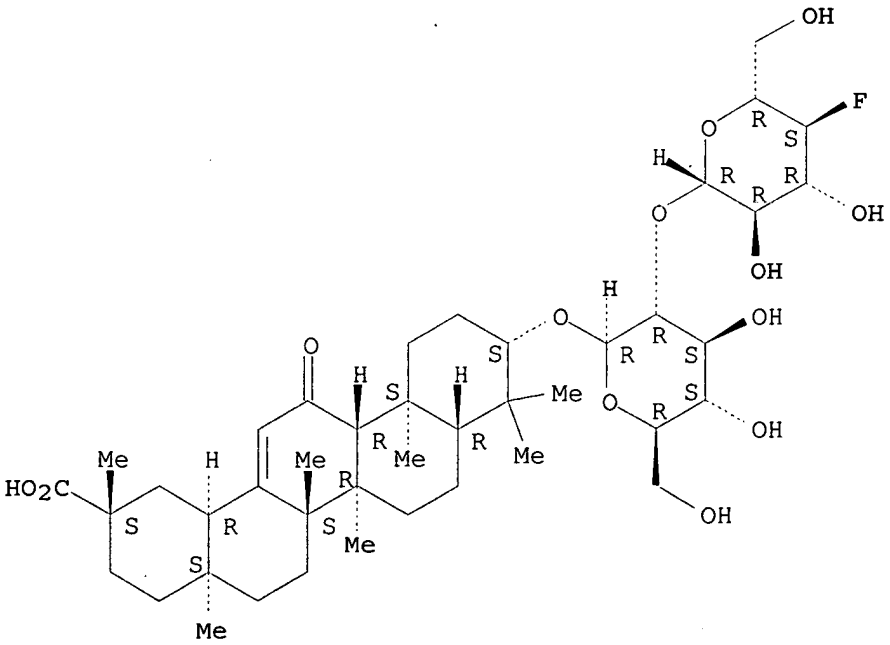
AB The inhibitory effects of several antiinflammatory agents, including glycyrrhizin (GL), on the activities of hyaluronidases (HAses) purified from bovine testes and Streptomyces were investigated in vitro. It was found that (i) GL inhibits the activity of HAse (p55) from bovine testes in a dose-dependent manner, but does not affect HAse from Streptomyces; (ii) GL was the most effective of the compds. tested on bovine testis HAse activity (50% inhibition with approx. 3 μM GL); and (iii) glycyrrhetinic acid (GA), a derivative (oGA) of GA and diglucuronic acid had no detectable effects on HAse activity at 9.0 μM. The GL-induced inhibition of HAse activity is uncompetitive for its substrates. Data are provided to support the contentions that (i) bovine testis HAse (p55) is a GL-binding protein; and (ii) GL acts as a potent inhibitor of HAse in vitro.

IT 187218-47-9
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(glycyrrhizin and other antiinflammatory agents as effective inhibitor for hyaluronidases from testis)

RN 187218-47-9 HCAPLUS

CN Olean-12-en-29-oic acid, 3-[[2-O-(4-deoxy-4-fluoro-β-D-glucopyranosyl)-β-D-glucopyranosyl]oxy]-11-oxo-, (3β,20β)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

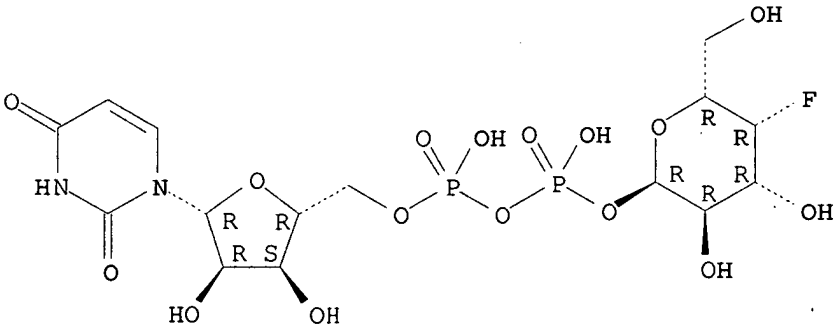
L24 ANSWER 16 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:589522 HCAPLUS
DOCUMENT NUMBER: 127:220925
TITLE: Preparation of fluorinated galactosyl nucleoside diphosphates to study the mechanism of the enzyme galactopyranose mutase
AUTHOR(S): Burton, Andrew; Wyatt, Paul; Boons, Geert-Jan
CORPORATE SOURCE: School of Chemistry, The University of Birmingham, Birmingham, B15 2TT, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1997), (16), 2375-2382
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 127:220925

AB A novel latent→active phosphorylation strategy has been employed for the preparation of two fluorinated nucleoside diphosphates. The strategy is based on the isomerization of substituted allyl to vinyl glycosides which were subsequently phosphorylated by treatment with dibenzyl hydrogen phosphate, N-iodosuccinimide and a catalytic amount of trimethylsilyl triflate. This methodol. is very suitable for the preparation of nucleoside diphosphates that have a modification in the saccharide moiety since the allyl moiety serves first as an anomeric protecting group, allowing for protecting-group manipulation and functionalization of the sugar ring, but after isomerization to the corresponding vinyl glycoside it acts as an anomeric leaving group. The 2-F and 4-F Gal-UDP derivs. do not inhibit the enzyme galactopyranose mutase in the direction pyranose → furanose but both compds. have been found to inhibit the reverse reaction.

IT 195147-58-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of fluorinated galactosyl nucleoside diphosphates to study the mechanism of the enzyme galactopyranose mutase)

RN 195147-58-1 HCAPLUS
CN Uridine 5'-(trihydrogen diphosphate), P'-(4-deoxy-4-fluoro-α-D-galactopyranosyl) ester, diammonium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



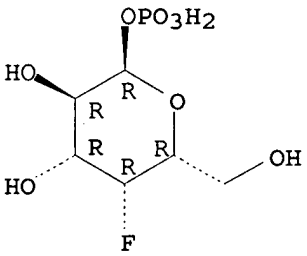
●2 NH_3

IT 195147-54-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of fluorinated galactosyl nucleoside diphosphates to study the mechanism of the enzyme galactopyranose mutase)
RN 195147-54-7 HCAPLUS
CN α-D-Galactopyranose, 4-deoxy-4-fluoro-, 1-(dihydrogen phosphate), compd. with N,N-diethylethanamine (1:2) (9CI) (CA INDEX NAME)

CM 1

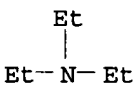
CRN 195147-53-6
CMF C6 H12 F O8 P

Absolute stereochemistry.



CM 2

CRN 121-44-8
CMF C6 H15 N



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

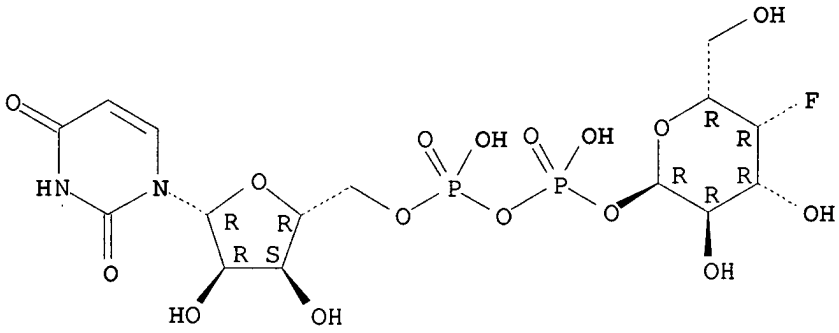
L24 ANSWER 17 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:297645 HCAPLUS
DOCUMENT NUMBER: 127:30827
TITLE: Structural Analysis of UDP-Sugar Binding to UDP-Galactose 4-Epimerase from Escherichia coli
AUTHOR(S): Thoden, James B.; Hegeman, Adrian D.; Wesenberg, Gary; Chapeau, Marie C.; Frey, Perry A.; Holden, Hazel M.
CORPORATE SOURCE: College of Agricultural and Life Sciences, University of Wisconsin at Madison, Madison, WI, 53705, USA
SOURCE: Biochemistry (1997), 36(21), 6294-6304
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB UDP-galactose 4-epimerase from Escherichia coli catalyzes the interconversion of UDP-galactose and UDP-glucose through the transient reduction of the tightly bound cofactor NAD+. The enzyme is unique among the NAD+-dependent enzymes in that it promotes stereospecific reduction of the cofactor but nonstereospecific hydride return during normal catalysis. In addition to hydride transfer, the reaction mechanism of epimerase involves two key features: the abstraction of a proton from the 4'-hydroxyl group

of glucose or galactose by an active site base and the rotation of a 4-ketopyranose intermediate in the active site pocket. To address the second issue of movement within the active site, the x-ray structures of reduced epimerase complexed with UDP-mannose, UDP-4-deoxy-4-fluoro-α-D-galactose, or UDP-4-deoxy-4-fluoro-α-D-glucose have been determined and refined to 1.65, 1.8, and 1.65 Å resolution, resp. A comparison of these models to that of the previously determined epimerase/NADH/UDP-glucose abortive complex reveals that the active site accommodates the various sugars by simple rearrangements of water mols. rather than by large changes in side chain conformations. In fact, the polypeptide chains for all of the epimerase/NADH/UDP-sugar complexes studied thus far are remarkably similar and can be superimposed with root-mean-square deviations of not greater than 0.24 Å. The only significant differences between the various enzyme/UDP-sugar models occur in two of the dihedral angles defining the conformation of the UDP-sugar ligands.

IT 190852-32-5D, UDP-galactose 4-epimerase complex
190852-34-7D, UDP-galactose 4-epimerase complex
RL: PRP (Properties)
(crystal structures of UDP-sugars binding to UDP-galactose 4-epimerase from Escherichia coli)

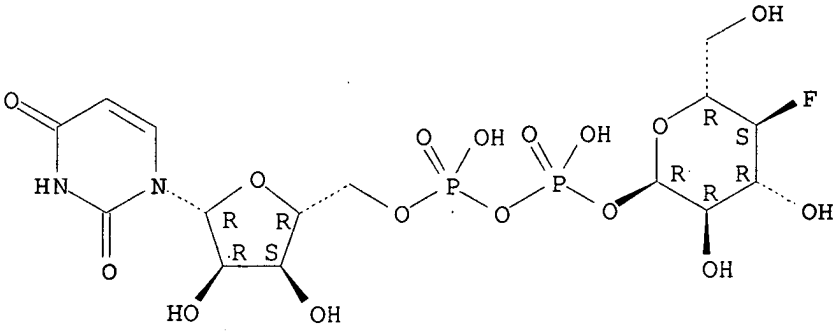
RN 190852-32-5 HCAPLUS
CN Uridine 5'-(trihydrogen diphosphate), P'-(4-deoxy-4-fluoro-α-D-galactopyranosyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 190852-34-7 HCAPLUS
CN Uridine 5'-(trihydrogen diphosphate), P'-(4-deoxy-4-fluoro-α-D-glucopyranosyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



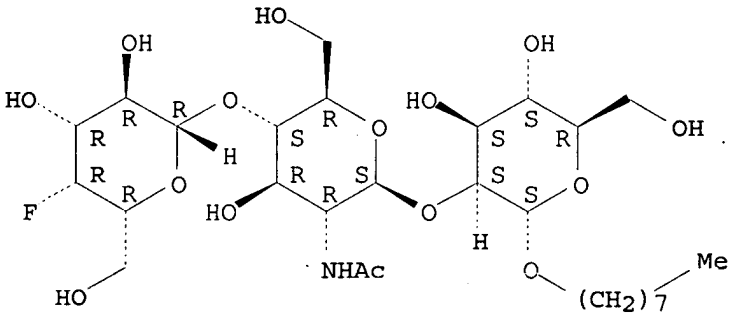
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 18 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:219271 HCAPLUS
DOCUMENT NUMBER: 126:251326
TITLE: Exploring the substrate specificity of sialyl-transferases
AUTHOR(S): van Dorst, Johannes A. L. M.; Kamerling, Johannis P.; Vliegenthart, Johannes F. G.
CORPORATE SOURCE: Dep. Bio-Organic Chem., Utrecht Univ., Utrecht, NL-3508, Neth.
SOURCE: Pure and Applied Chemistry (1997), 69(3), 537-542
CODEN: PACHAS; ISSN: 0033-4545
PUBLISHER: Blackwell
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Twelve trisaccharide derivs. designed for detailed exploration of the acceptor specificity of sialyltransferases involved in the biosynthesis of N-glycans have been synthesized. These compds. include β-D-Galp-(1-4)-β-D-GlcpNAc-(1-2)-α-D-Manp-(1-O)(CH2)7CH3 and analogs containing structural variants of D-galactose. All trisaccharides were obtained by condensation of suitably modified glycosyl donors with a single disaccharide acceptor, thus limiting the number of reaction steps required. After deprotection, the compds. were employed to delineate the recognition characteristics of several natural and recombinant sialyltransferases.

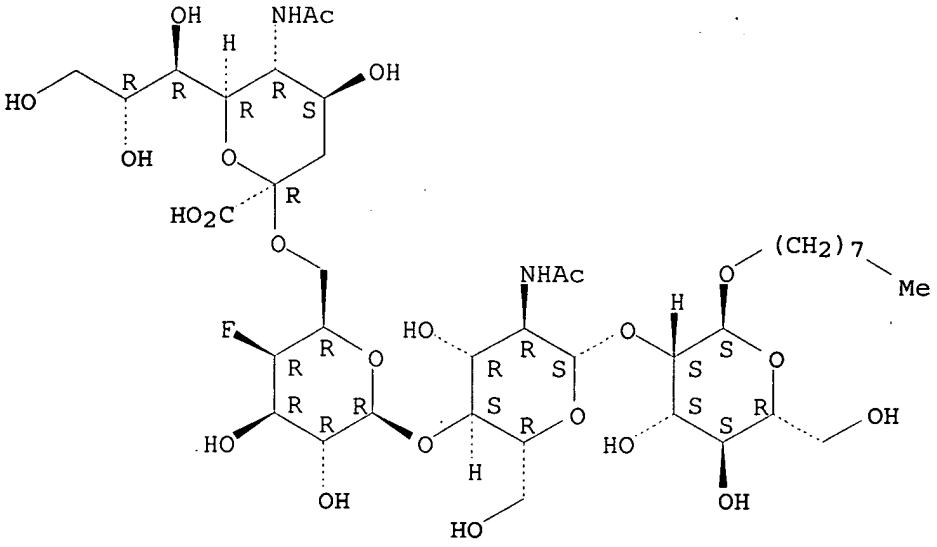
IT 183292-98-0P
RL: BPR (Biological process); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(substrate specificity of sialyl-transferases via sialylation of trisaccharides)
RN 183292-98-0 HCAPLUS
CN α-D-Mannopyranoside, octyl O-4-deoxy-4-fluoro-β-D-galactopyranosyl-(1→4)-O-2-(acetylamino)-2-deoxy-β-D-glucopyranosyl-(1→2)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 188685-49-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(substrate specificity of sialyl-transferases via sialylation of trisaccharides)
RN 188685-49-6 HCAPLUS
CN α-D-Mannopyranoside, octyl O-(N-acetyl-α-neuraminosyl)-(2→6)-O-4-deoxy-4-fluoro-β-D-galactopyranosyl-(1→4)-O-2-(acetylamino)-2-deoxy-β-D-glucopyranosyl-(1→2)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

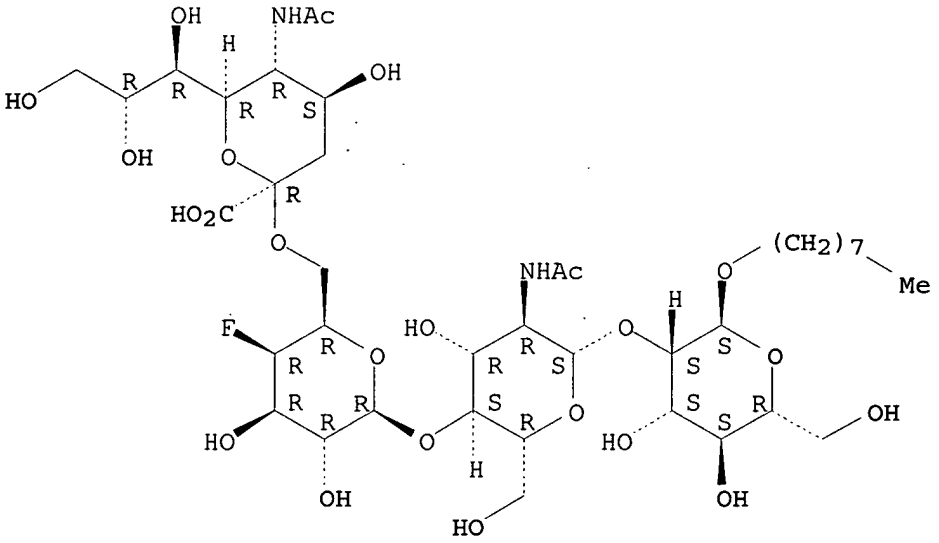
L24 ANSWER 19 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:55762 HCAPLUS
DOCUMENT NUMBER: 126:260759
TITLE: Exploring the substrate specificities of α-2,6- and α-2,3-sialyltransferases using synthetic acceptor analogs
AUTHOR(S): Van Dorst, Jahannes A. L. M.; Tikkanen, Jaana M.; Krezdorn, Christian H.; Streiff, Markus B.; Berger, Eric G.; Van Kuik, J. Albert; Kamerling, Johannis P.; Vliegenthart, Johannes F. G.
CORPORATE SOURCE: Bijvoet Center, Utrecht University, Utrecht, 3508 TB, Neth.
SOURCE: European Journal of Biochemistry (1996), 242(3), 674-681
CODEN: EJBCAI; ISSN: 0014-2956
PUBLISHER: Springer
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:260759

AB The acceptor specificities of rat liver Gal(/β1-4)GlcNAc α-2,6-sialyltransferase, recombinant full-length human liver Gal(β1-4)GlcNAcα-2,6-sialyltransferase, and a soluble form of recombinant rat liver Gal(β1-3/4)GlcNAc α-2,3-sialyltransferase were studied with analogs of the trisaccharide Gal(β1-4)GlcNAc(β1-2)Man(α1-O)(CH2)7CH3. These analogs contain structural variants of r0-galactose, modified at either C3, C4 or C5 by deoxygenation, fluorination, O-methylation, epimerization, or by the introduction of an amino group. In addition, the enantiomer of D-galactose is included. The α-2,6-sialyltransferases tolerated most of the modifications at the galactose residue to some extent, whereas the α-2,3-sialyltransferase displayed a narrower specificity. Mol. dynamics simulations were performed to correlate enzymic activity to 3-dimensional structure. Ineffective acceptors for rat liver c-2,6-sialyltransferase were inhibitory towards the enzyme; likewise, the α-2,3-sialyltransferase was inhibited by all non-substrates. Modified sialyloligosaccharides were obtained on a mg scale by incubation of effective acceptors with 1 of each of the 3 enzymes, and characterized by 500-MHz 1H-NMR spectroscopy.

IT 188685-49-6P

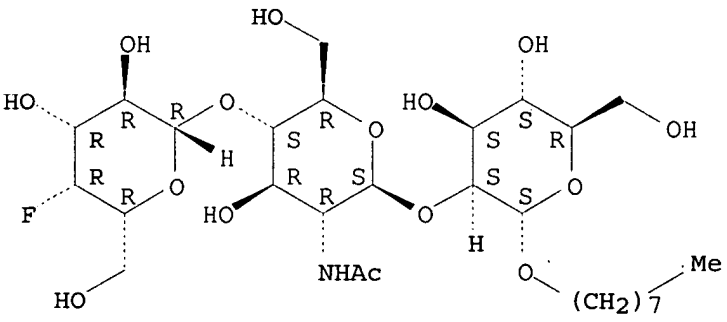
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(sialyloligosaccharides synthesized by α-2,6- and α-2,3-sialyltransferases)
RN 188685-49-6 HCAPLUS
CN α-D-Mannopyranoside, octyl O-(N-acetyl-α-neuraminosyl)-(2→6)-O-4-deoxy-4-fluoro-β-D-galactopyranosyl-(1→4)-O-2-(acetylamino)-2-deoxy-β-D-glucopyranosyl-(1→2)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 183292-98-0
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(α-2,6- and α-2,3-sialyltransferases substrate specificities studied by synthetic acceptor analogs)
RN 183292-98-0 HCAPLUS
CN α-D-Mannopyranoside, octyl O-4-deoxy-4-fluoro-β-D-galactopyranosyl-(1→4)-O-2-(acetylamino)-2-deoxy-β-D-glucopyranosyl-(1→2)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L24 ANSWER 20 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:49061 HCAPLUS
DOCUMENT NUMBER: 126:171785
TITLE: Synthesis of glycyrrhizin analogs containing

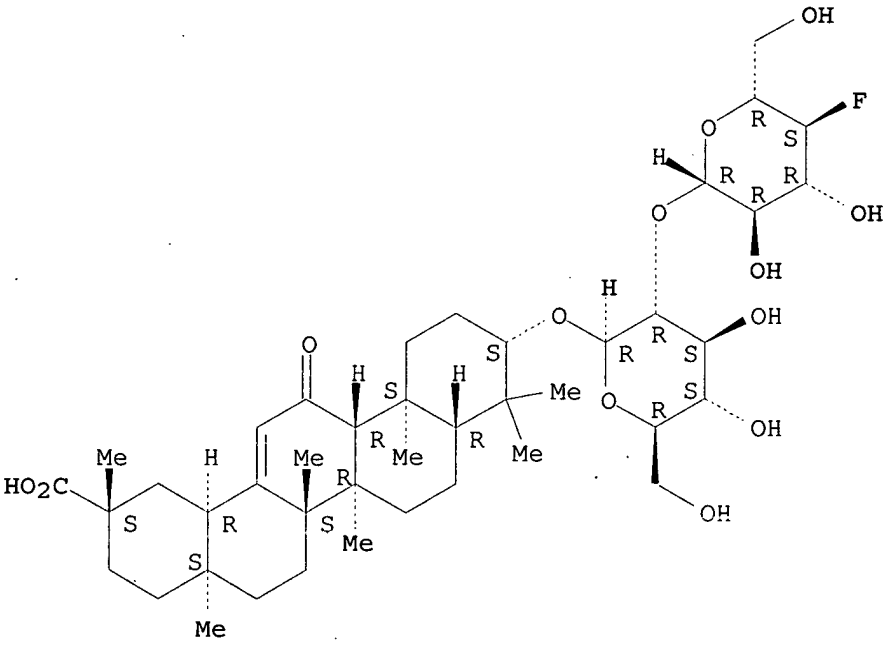
fluorinated β(1→2)-linked disaccharides
AUTHOR(S): Morishima, Naohiko; Mori, Yoko
CORPORATE SOURCE: Sch. of Nursing, Kitasato Univ., 228, Japan
SOURCE: Bioorganic & Medicinal Chemistry (1996), 4(11), 1799-1808
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB For studies on the recognition mechanisms for glycyrrhizin-induced biol. activities, seven Glycyrrhizin analogs with 3'-, 4'-, 6'-, 3-, and 4-fluorinated 2-O-β-D-glucopyranosyl-β-D-glucopyranoses and 3- and 4-fluorinated 2-O-β-D-glucopyranuronosyl-β-D-glucopyranoses were synthesized through a stepwise glycosidation procedure. 1,2-Di-O-acetyl-4,6-di-O-benzyl-3-deoxy-3-fluoro- and 1,2-di-O-acetyl-3,6-di-O-benzyl-4-deoxy-4-fluoro-D-glucopyranose were employed for the first β-glycosidation of Me glycyrrhetate, promoted with trimethylsilyl trifluoromethanesulfonate.

IT 187218-47-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of glycyrrhizin analogs containing fluorinated β(1→2)-linked disaccharides)

RN 187218-47-9 HCAPLUS
CN Olean-12-en-29-oic acid, 3-[[2-O-(4-deoxy-4-fluoro-β-D-glucopyranosyl)-β-D-glucopyranosyl]oxy]-11-oxo-, (3β,20β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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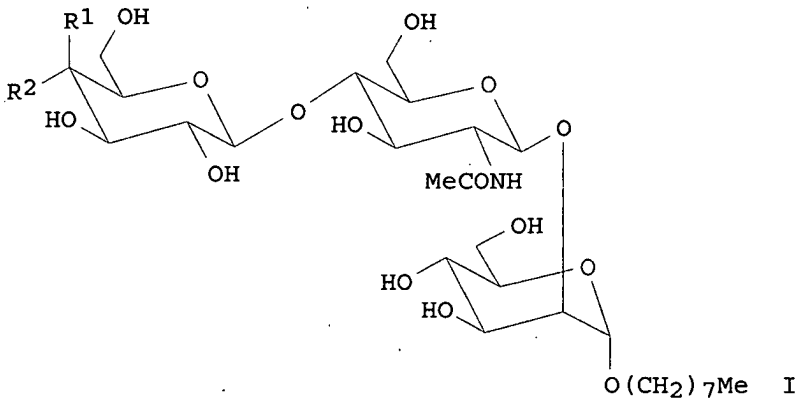
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jan 11, 2008 (20080111/UP).

=> d l24 ibib abs hitstr 21-30
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:y

L24 ANSWER 21 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:611534 HCAPLUS
DOCUMENT NUMBER: 125:329152
TITLE: Synthesis of hexp-(1→4)-β-D-GlcpNAc-(1→2)-α-D-Manp-(1→O)(CH2)7CH3 probes for exploration of the substrate specificity of glycosyltransferases. Part I. Hex = β-D-Gal, 4-deoxy-β-D-Gal, 4-O-methyl-β-D-Gal, 4-deoxy-4-fluoro-β-D-Gal, or β-D-Glc
AUTHOR(S): van Dorst, Johannes A. L. M.; van Heusden, Cornelis J.; Voskamp, Anton F.; Kamerling, Johannis P.; Vliegenthart, Johannes F. G.
CORPORATE SOURCE: Department Bio-Organic Chemistry, Utrecht University, Utrecht, NL-3508, Neth.
SOURCE: Carbohydrate Research (1996), 291, 63-83
CODEN: CRBRAT; ISSN: 0008-6215
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

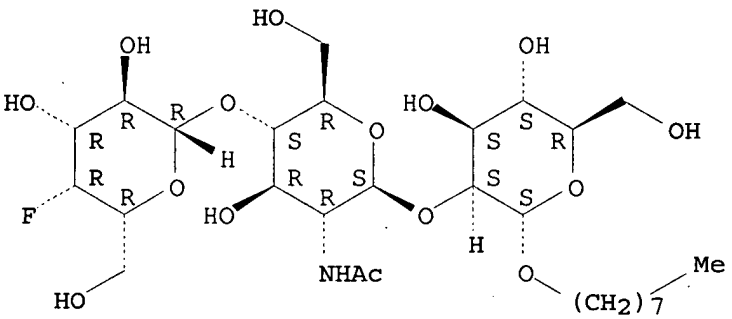
AB Five trisaccharide derivs. designed for detailed exploration of the acceptor specificity of glycosyltransferases involved in termination of N-acetyllactosamine-type structures were synthesized: β-D-Galp-(1→4)-β-D-GlcpNAc-(1→2)-α-D-Manp-(1→O)(CH2)7CH3, 4-deoxy-β-D-Galp-(1→4)-β-D-GlcpNAc-

(1→2)-α-D-Manp-(1→O)(CH2)7CH3, 4-O-methyl-β-D-Gal p-(1→4)-β-D-GlcpNAc-(1→2)-α-D-Manp-(1→O)(CH2)7CH3, 4-deoxy-4-fluoro-β-D-Galp-(1→4)-β-D-GlcpNAc-(1→2)-α-D-Manp-(1→O)(CH2)7CH3, and β-D-Glcp-(1→4)-β-D-GlcpNAc-(1→2)-α-D-Manp-(1→O)(CH2)7CH3. A general disaccharide acceptor octyl 3,4,6-tri-O-benzyl-2-O-(3,6-di-O-benzyl-2-deoxy-2-phthalimido-β-D-glucopyranosyl)-α-D-mannopyranoside was synthesized by condensation of 4-O-acetyl-3,6-di-O-benzyl-2-deoxy-2-phthalimido-α-D-glucopyranosyl trichloroacetimidate with octyl 3,4,6-tri-O-benzyl-α-D-mannopyranoside, followed by deacetylation. 2,3,4,6-Tetra-O-acetyl-α-D-galactopyranosyl trichloroacetimidate and 2,3,4,6-tetra-O-acetyl-α-D-glucopyranosyl trichloroacetimidate were used as glycosyl donors in the synthesis of the compds. above. The target compds. were derivs. and analogs of I (R1 = OH, H, OMe, F; R2 = H, OH).

IT 183292-98-0P
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(preparation of octyl (galactopyranosyl)(glucopyranosyl)mannopyranoside and analogs as probes for glycosyltransferase substrate specificity)

RN 183292-98-0 HCAPLUS
CN α-D-Mannopyranoside, octyl O-4-deoxy-4-fluoro-β-D-galactopyranosyl-(1→4)-O-2-(acetylamino)-2-deoxy-β-D-glucopyranosyl-(1→2)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L24 ANSWER 22 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:471933 HCAPLUS
DOCUMENT NUMBER: 125:329142
TITLE: 4-Deoxy-analogs of p-nitrophenyl β-D-galactopyranosides for specificity study with β-galactosidase from Escherichia coli
AUTHOR(S): Yoon, Shinsook; Kim, Hyoung Geun; Chun, Keun Ho; Shan, Jeong E. Nam
CORPORATE SOURCE: Dep. Chem., Soong Sil Univ., Seoul, 156-743, S. Korea
SOURCE: Bulletin of the Korean Chemical Society (1996), 17(7), 599-604
CODEN: BKCSDE; ISSN: 0253-2964
PUBLISHER: Korean Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

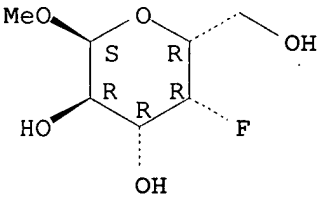
AB The synthesis is reported of p-nitrophenyl glycosides of D-galactose modified at C-4 with azido- (5), amino- (6) group and fluorine (13). 4-Azido-2,3,6-tri-O-benzoyl-4-deoxy-α-D-galactopyranosyl chloride and 2,3,6-tri-O-benzoyl-4-deoxy-4-fluoro-α-D-galactopyranosyl bromide were coupled with potassium p-nitrophenoxide in the presence of 18-crown-6-giving the corresponding p-nitrophenyl 4-azido- and

4-fluoro-4-deoxy-β-D-galactopyranoside derivs. P-Nitrophenyl 4-amino-4-deoxy-β-D-galactopyranoside was obtained by selective reduction of p-nitrophenyl 4-azido-4-deoxy-β-D-galactopyranoside using 1,3-propane dithioltriethylamine. These galactoside analogs were slowly hydrolyzed by β-galactosidase from Escherichia coli.

IT 32934-07-9P 183552-00-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and β-galactosidase-catalyzed hydrolysis of 4-deoxy-analogs of p-nitrophenyl β-galactopyranosides)

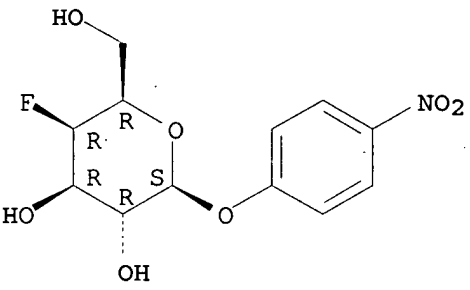
RN 32934-07-9 HCAPLUS
CN α-D-Galactopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 183552-00-3 HCAPLUS
CN β-D-Galactopyranoside, 4-nitrophenyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L24 ANSWER 23 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:448941 HCAPLUS
DOCUMENT NUMBER: 125:152289
TITLE: Enthalpy of solution of carbohydrates using a modified differential scanning calorimeter
AUTHOR(S): Schwarz, Frederick P.
CORPORATE SOURCE: Cent. Adv. Res. Biotechnol., Natl. Inst. Stand. Technol., Rockville, MD, 20850, USA
SOURCE: Journal of Solution Chemistry (1996), 25(5), 471-484
CODEN: JSLCAG; ISSN: 0095-9782
PUBLISHER: Plenum
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A differential scanning calorimeter (DSC) was modified for the determination of enthalpies of solution The measurements were performed on aqueous solns. of the deoxy- and fluoro-deoxy derivs. of D-glucopyranose (Glu) where the OH group on the C1, C2, C3, and C6 is replaced by H (1HGlu, 2HGlu, 3HGlu, and 6HGlu) and by F (1FGlu, 2FGlu, 3FGlu, and 6FGlu), 4-deoxy-4-fluoro-α-D-glucopyranoside (4FGlu), 1-methoxy-α-D-glucopyranoside

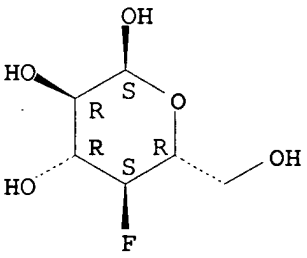
(αMeOGlu), 1-phenoxy-α-D-glucopyranoside (αPheOGlu), D-mannopyranose (Man), and 3-methoxy-α-D-glucopyranoside (3MeOGlu) at 15.1, 25.0, 35.0, and 45.1°C. The enthalpies of soln ΔsH0(T) ranged from 1.00 ± 0.25 kJ-mol-1 for 6HGlu at 15.1°C to 20.4±1.4 for αPhOGlu at 45.1°C and were in good agreement with literature values for man, αGlu, αMeOGlu, and 3MeOGlu at 25.0 and 35.0°C and for αMeOMan and 2HGlu at 35.0°C. ΔsH0(T) for the derivs. were then extrapolated up to the melting temperature Tm and compared wit their enthalpies of fusion, ΔfH, also determined from DSC measurements. If the agreement between ΔsH0(Tm) and ΔfH was within the 95% confidence level, then it was concluded that intermol. interactions between the carbohydrate mols. in the liquid phase were the same as between the carbohydrate and water mols. in the solution phase. This agreement was observed for aqueous solns. of Man, αGlu, αMeOGlu, 3HGlu, 3FGlu, and 6FGlu.

IT 62182-11-0
RL: PRP (Properties)
(enthalpies of solution and fusion of carbohydrates measured using modified differential scanning calorimeter)

RN 62182-11-0 HCAPLUS

CN α-D-Glucopyranose, 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 24 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:335058 HCAPLUS

DOCUMENT NUMBER: 125:28519

TITLE: Different architecture of the combining site of the two chicken galectins revealed by chemical mapping studies with synthetic ligand derivatives

AUTHOR(S): Solis, Dolores; Romero, Antonio; Kaltner, Herbert; Gabius, Hans-Joachim; Diaz-Maurino, Teresa

CORPORATE SOURCE: Inst. Qium. Fis. Rocasolano, Consejo Super. Investigaciones Cientificas, Madrid, E-28006, Spain

SOURCE: Journal of Biological Chemistry (1996), 271(22), 12744-12748
CODEN: JBCHA3; ISSN: 0021-9258

PUBLISHER: American Society for Biochemistry and Molecular Biology

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The detailed comparison of the carbohydrate-binding properties of related galectins from one organism can be facilitated by the application of an array of deliberately tailored Me β-lactoside derivs. Focusing on chicken due to its expression of two galectins as a model for this approach, the combining-site architecture of the lectin from adult liver (CL-16) is apparently homologous to that previously observed for bovine galectin-1 (Solis, D., Jimenez-Barbero, J., Martin-Lomas, M., and Diaz-Maurino, T. (1994) Eur. J. Biochem. 223, 107-114). Besides preservation of the key interactions and minor differences, the lectin from adult intestine (CL-14) is able to accommodate an axial HO-3 at the

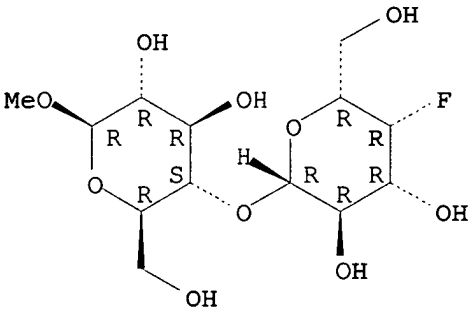
glucose moiety. Homol.-based modeling enabled us to tentatively attribute the observed differences to a slightly different orientation of pivotal side chains in the binding pocket due to distinct substitutions of amino acid residues in the variable region within the carbohydrate-recognition domain. Thus, the results suggest overlapping but distinct ranges of potential ligands for the two chicken lectins and provide new information on their relationship to mammalian galectins. The described approach is suggested to be of relevance to design pharmaceuticals with enhanced selectivity to a certain member within a family of related lectins.

IT 149457-67-0
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(binding of by galectin; carbohydrate-binding specificities of two chicken galectins revealed by chemical mapping studies with synthetic carbohydrate derivs.)

RN 149457-67-0 HCAPLUS

CN β-D-Glucopyranoside, methyl 4-O-(4-deoxy-4-fluoro-β-D-galactopyranosyl)- (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 25 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:325042 HCAPLUS

DOCUMENT NUMBER: 125:3900

TITLE: Effect of substituent on the thermodynamics of D-glucopyranoside binding to concanavalin A, pea (Pisum sativum) lectin and lentil (Lens culinaris) lectin

AUTHOR(S): Schwarz, Frederick P.; Misquith, Sandra; Surolia, Avadhesha

CORPORATE SOURCE: Cent. Adv. Res. Biotechnology, Natl. Inst. Standards and Technology, Rockville, MD, 20850, USA

SOURCE: Biochemical Journal (1996), 316(1), 123-129
CODEN: BIJOAK; ISSN: 0264-6021

PUBLISHER: Portland Press

DOCUMENT TYPE: Journal

LANGUAGE: English

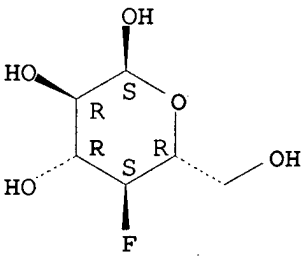
AB Titration calorimetry measurements of the binding of phenyl-α (αPhOGlu), 3-methoxy (3MeOGlu), fluorodeoxy and deoxy derivs. of α-D-glucopyranose (Glu) to Con A (conAd), pea lectin and lentil lectin were performed at approx. 10 and 25° in 0.01 M dimethylglutaric acid/NaOH buffer, pH 6.9, containing 0.15 M NaCl and Mn2+ and Ca2+ ions. Apparently the 3-deoxy, 4-deoxy and 6-deoxy as well as the 4-fluorodeoxy and 6-fluorodeoxy derivs. of Glu do not bind to the lectins because no heat release was observed on the addition of aliquots of solns. of these derivs. to the lectin solns. The binding enthalpies, ΔH0b, and entropies, ΔS0b, determined from the measurements were compared with the same thermodn. binding parameters for Glu, D-mannopyranoside and methyl-α-D-glucopyranoside (αMeOGlu). The binding reactions

are enthalpically driven with little change in the heat capacity on binding, and exhibit enthalpy-entropy compensation. Differences between the thermodn. binding parameters can be rationalized in terms of the interactions apparent in the known crystal structures of the methyl-α-D-mannopyranoside-conA [Derewenda, Yariv, Helliwell, Kalb (Gilboa), Dodson, Papiz, Wan and Campbell (1989) EMBO J. 8, 2189-2193] and pea lectin-trimannopyranoside [Rini, Hardman, Einspahr, Suddath and Carber (1993) J. Biol. Chemical 268, 10126-10132] complexes. Increases in the entropy change on binding are observed for αMeOGlu binding to pea and lentil lectin, for αPhOGlu binding to conA and pea lectin, and for 3MeOGlu binding to pea lectin relative to the entropy change for Glu binding, and imply that the phenoxy and methoxy substituents provide addnl. hydrophobic interactions in the complex. Increases in the binding enthalpy relative to that of Glu are observed for deoxy and fluoro derivs. in the C-1 and C-2 positions and imply that these substituents weaken the interaction with the surrounding water, thereby strengthening the interaction with the binding site.

IT 62182-11-0
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(effect of substituent on thermodn. of D-glucopyranoside binding to Con A, pea (Pisum sativum) lectin and lentil (Lens culinaris) lectin)

RN 62182-11-0 HCAPLUS
CN α-D-Glucopyranose, 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 26 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:945146 HCAPLUS
DOCUMENT NUMBER: 124:24613
TITLE: Mechanism of Agrobacterium β-glucosidase: kinetic analysis of the role of noncovalent enzyme/substrate interactions
AUTHOR(S): Namchuk, Mark N.; Withers, Stephen G.
CORPORATE SOURCE: Department of Chemistry, University of British Columbia, Vancouver, BC, V6T 1Z1, Can.
SOURCE: Biochemistry (1995), 34(49), 16194-202
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

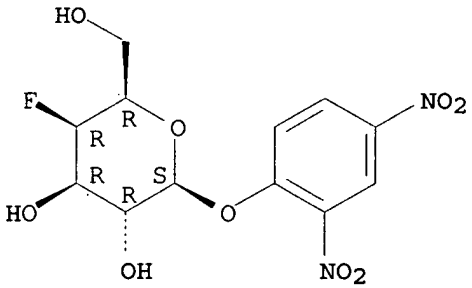
AB The role of noncovalent interactions in the catalytic mechanism of the A. faecalis β-glucosidase was investigated by steady-state and pre-steady state kinetic anal. of the hydrolysis of a series of monosubstituted aryl glycosides, in which the OH groups on the glycone were substituted by H or F. The contributions of each OH group to binding of these substrates at the ground state were relatively weak (interaction energies of 3.3 kJ/mol or smaller) but were much greater at the 2 transition states (glycosylation and deglycosylation). The strongest transition state interactions were at the 2 position (at least 18 and 22 kJ/mol for glycosylation and deglycosylation, resp.) with the interactions

at the 3 and 6 positions contributing at least another 9 kJ/mol of binding energy at both transition states. The interaction at the 4 position was less crucial to transition state binding but important for stabilization of the glycosyl-enzyme intermediate. Comparison of observed rates with those for spontaneous hydrolysis of the same substrates provided evidence for oxocarbenium ion character at both transition states, that for deglycosylation apparently having the greater pos. charge development at the anomeric center.

IT 144220-98-4 171626-62-3
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(preparation of substrate analogs for kinetic studies of β-glucosidase from Agrobacterium faecalis)

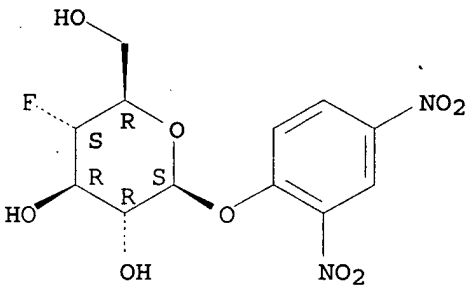
RN 144220-98-4 HCAPLUS
CN β-D-Galactopyranoside, 2,4-dinitrophenyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



RN 171626-62-3 HCAPLUS
CN β-D-Glucopyranoside, 2,4-dinitrophenyl 4-deoxy-4-fluoro- (CA INDEX NAME)

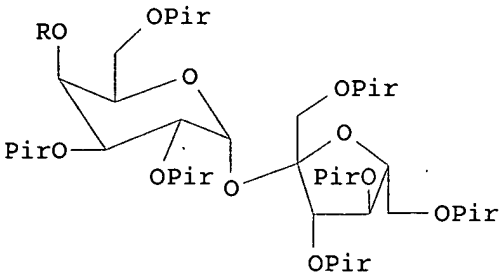
Absolute stereochemistry.



L24 ANSWER 27 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER:	1995:766557 HCAPLUS
DOCUMENT NUMBER:	124:9168
TITLE:	Synthesis of sucrose analogs modified at position 4
AUTHOR(S):	Simiand, Cecile; Driguez, Hugues
CORPORATE SOURCE:	Centre Recherches Macromolecules Vegetales, Grenoble, 38041, Fr.
SOURCE:	Journal of Carbohydrate Chemistry (1995), 14(7), 977-83 CODEN: JCACDM; ISSN: 0732-8303
PUBLISHER:	Dekker
DOCUMENT TYPE:	Journal
LANGUAGE:	English

GI



I

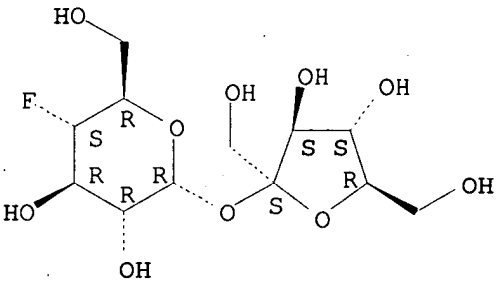
AB Treatment of 1,3,4,5-tetra-O-pivaloyl-β-D-fructofuranosyl 2,3,6-tri-O-pivaloyl-4-O-triflyl-α-D-glucopyranoside with sodium nitrite gave the galacto-sucrose heptapivalate I (R = H) in high yield. This compound was converted into 4-deoxy-4-fluorosucrose heptapivalate by treatment with DAST. The reaction of triflate I (R = CF3SO2) (II) with lithium azide gave 4-azido-4-deoxysucrose heptapivalate which was transformed into 4-amino-4-deoxysucrose by deacylation and hydrogenation. SN2 displacement of the triflate of II with thioacetate ion provided the expected 4-S-acetyl-4-thiosucrose heptapivalate in excellent yield. The latter compound on deacylation gave a mixture of 4-thiosucrose and 4-thiosucrose disulfide.

IT 171339-45-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of sucrose analogs modified at position 4)

RN 171339-45-0 HCAPLUS

CN α-D-Glucopyranoside, β-D-fructofuranosyl 4-deoxy-4-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 28 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:748183 HCAPLUS

DOCUMENT NUMBER: 123:192044

TITLE: Substrate specificity of small-intestinal lactase: study of the steric effects and hydrogen bonds involved in enzyme-substrate interaction

AUTHOR(S): Fernandez, Paloma; Canada, F. Javier; Jimenez-Barbero, Jesus; Martin-Lomas, Manuel

CORPORATE SOURCE: Inst. Quim. Org., Consejo Superior Invest. Cientificas, Madrid, 28006, Spain

SOURCE: Carbohydrate Research (1995), 271(1), 31-42
CODEN: CRBRAT; ISSN: 0008-6215

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

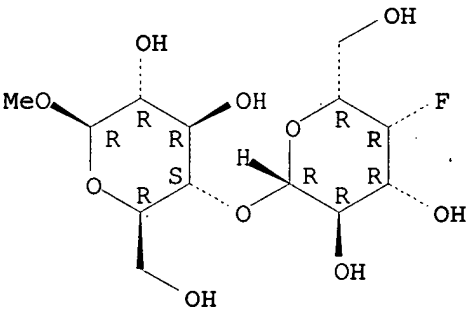
AB Milk lactose is hydrolyzed to D-galactose and D-glucose in the small intestine of mammals by the lactase-phlorizin hydrolase complex (LPH, EC 3.2.1.23-62). Lactase activity has broad substrate selectivity and several glycosides are substrates. Recently, using the monodeoxy derivs. of Me β-lactoside (1), the authors have shown the importance of each hydroxyl group in the substrate mol. concerning the interaction with the enzyme. Now the authors have studied the corresponding O-Me derivs., as well as some of the halo derivs. of 1. The authors have found that the enzyme presents steric restrictions to the recognition of substrates modified in the galactose moiety. In contrast, the binding site for the aglycon part of the substrate is looser. The authors have previously shown that HO-3' and HO-6 were important for the recognition of the substrate by the enzyme. Now the authors have found that the corresponding fluorine derivs. are not, or very poorly, recognized. This suggests that the HO-3' and HO-6 participate, as donors, in hydrogen bonds in the interaction with the enzyme.

IT 149457-67-0
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(substrate specificity of small-intestinal lactase and study of steric effects and hydrogen bonds involved in enzyme-substrate interaction)

RN 149457-67-0 HCAPLUS

CN β-D-Glucopyranoside, methyl 4-O-(4-deoxy-4-fluoro-β-D-galactopyranosyl)- (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 29 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:178156 HCAPLUS

DOCUMENT NUMBER: 122:26531

TITLE: Synthesis of UDP-4-deoxy-4-fluoroglucose and UDP-4-deoxy-4-fluorogalactose and their Interactions with Enzymes of Nucleotide Sugar Metabolism

AUTHOR(S): Chapeau, Marie-Christine; Frey, Perry A.

CORPORATE SOURCE: Institute for Enzyme Research, University of Wisconsin-Madison, Madison, WI, 53705, USA

SOURCE: Journal of Organic Chemistry (1994), 59(23), 6994-8
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Fluorinated carbohydrates can be used as probes of enzymic active sites. The authors report the synthesis of 4-deoxy-4-fluoro-α-D-galactose-1-phosphate and the substrate analogs of UDP-galactose, UDP-4-deoxy-4-fluoro-α-D-galactose (UDP-FGal), and of UDP-glucose, UDP-4-deoxy-4-fluoro-α-D-glucose (UDP-FGlc), which may be useful in analyzing the binding properties of enzymes that utilize nucleotide sugars as substrates. As a first step in this study, the authors determine the kinetic and inhibition

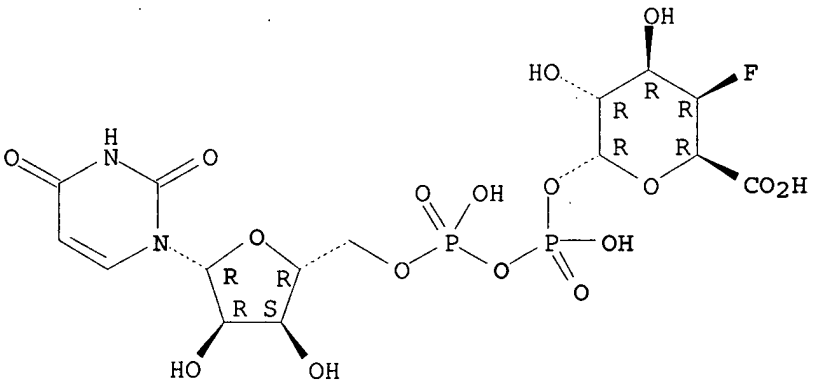
parameters for UDP-FGal and UDP-FGlc interacting with UDP-glucose dehydrogenase and UDP-galactose 4-epimerase. UDP-FGlc is a substrate for bovine liver UDP-glucose dehydrogenase: Km = 30.2 μM slightly higher than the value 9.6 μM for UDP-glucose, and VmUDP-FGlc = 0.46VmUDP-Glc. UDP-FGal is not a substrate for UDP-glucose dehydrogenase but is a competitive inhibitor with respect to UDP-glucose (Ki = 19.9 μM). These analogs also bind to UDP-galactose 4-epimerase from E. coli with dissociation consts. Kd of 1.4 and 1.1 mM for UDP-FGlc and UDP-FGal, resp.

IT 159758-91-5P
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(preparation of UDP-4-deoxy-4-fluorogalactose and its interactions with UDP-glucose dehydrogenase and UDP-galactose 4-epimerase)

RN 159758-91-5 HCAPLUS

CN α-D-Galactopyranuronic acid, 4-deoxy-4-fluoro-, 1→P'-ester with uridine 5'-(trihydrogen diphosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

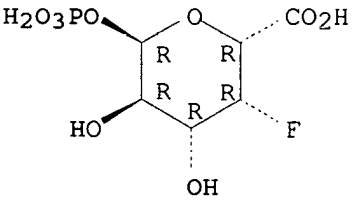


IT 159758-92-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of UDP-4-deoxy-4-fluorogalactose and its interactions with UDP-glucose dehydrogenase and UDP-galactose 4-epimerase)

RN 159758-92-6 HCAPLUS

CN α-D-Galactopyranuronic acid, 4-deoxy-4-fluoro-, 1-(dihydrogen phosphate) (CA INDEX NAME)

Absolute stereochemistry.

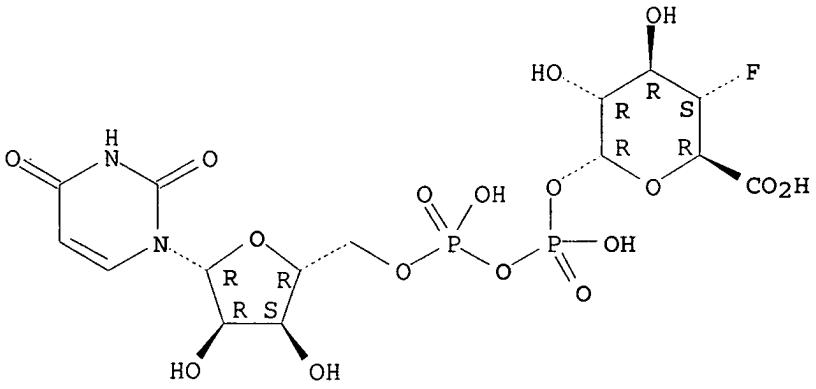


IT 159758-90-4P
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(preparation of UDP-4-deoxy-4-fluoroglucose and its interactions with UDP-glucose dehydrogenase and UDP-galactose 4-epimerase)

RN 159758-90-4 HCAPLUS

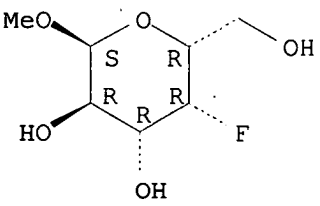
CN α-D-Glucopyranuronic acid, 4-deoxy-4-fluoro-, 1→P'-ester with uridine 5'-(trihydrogen diphosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 30 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:16079 HCAPLUS
DOCUMENT NUMBER: 122:106285
TITLE: Synthesis of specifically monofluorinated ligands related to the O-polysaccharide of Shigella dysenteriae type 1
AUTHOR(S): Mulard, Laurence A.; Kovac, Paul; Glaudemans, Cornelis P. J.
CORPORATE SOURCE: NIDDK, National Institutes of Health, Bethesda, MD, USA
SOURCE: Carbohydrate Research (1994), 259(1), 21-34
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis is reported of galactopyranose nucleophiles monofluorinated at positions 3, 4, or 6 and protected by 4,6-O-benzylidene, 3,6-di-O-benzyl, or 3,4-O-isopropylidene groups, resp. The condensation of these nucleophiles with 2,3,4-tri-O-benzoyl-α-L-rhamnosyl bromide gave, after deprotection, the disaccharide analogs of Me O-α-L-rhamnopyranosyl-(1→2)-α-D-galactopyranoside, monofluorinated at position 3, 4, or 6 of the galactoside residue.
IT 32934-07-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of monofluorinated ligands related to the O-polysaccharide of Shigella dysenteriae)
RN 32934-07-9 HCAPLUS
CN α-D-Galactopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



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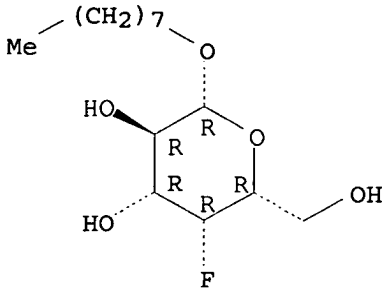
L24 ANSWER 31 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:476994 HCAPLUS
DOCUMENT NUMBER: 121:76994
TITLE: Recognition of synthetic analogs of the acceptor, β-D-Galp-OR, by the blood-group H gene-specified glycosyltransferase
AUTHOR(S): Lowary, Todd L.; Swiedler, Stuart J.; Hindsgaul, Ole
CORPORATE SOURCE: Department of Chemistry, University of Alberta, Edmonton, Alberta, Can.
SOURCE: Carbohydrate Research (1994), 256(2), 257-73
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The acceptor-substrate specificity of a cloned α-(1→2) fucosyltransferase has been explored using structural analogs of octyl β-D-galactopyranoside (I). This monosaccharide is the min. acceptor-substrate for the H-transferase, one of two enzymes responsible for the biosynthesis of the O blood-group antigen, which terminates in the sequence α-L-Fucp-(1→2)-β-D-Galp. Galactoside I has a Km of 6 mM with this enzyme. Eighteen analogs of I have been prepared, including those where the hydroxyl groups at C-3, C-4, and C-6 have been replaced, independently, with deoxy, fluoro, O-Me, amino, and acetamido functionalities. The C-3 and C-4 epimers have been prepared as has the C-5 de(hydroxymethyl)ated derivative These compds. were screened as potential acceptors and inhibitors of the fucosyltransferase. The C-6 analogs that do not possess a charge show substrate activity with relative rates in the range of 27-316% that of I. The C-3 modified analogs are inhibitors with estimated Ki values of 0.9-43 mM. Those analogs with modifications at C-4 were both poor inhibitors and acceptors.

IT 156570-26-2
RL: BIOL (Biological study)
(human blood group H fucosyltransferase reaction with, structure in relation to)
RN 156570-26-2 HCAPLUS
CN β-D-Galactopyranoside, octyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.

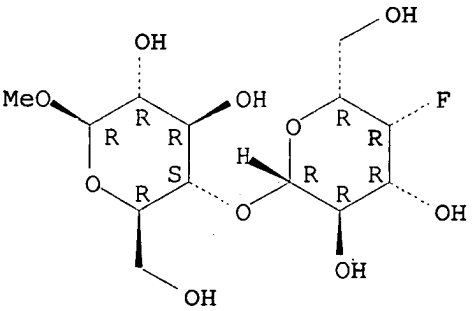


L24 ANSWER 32 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:436028 HCAPLUS
DOCUMENT NUMBER: 121:36028
TITLE: Syntheses of all the possible monomethyl ethers and several deoxyhalo analogs of methyl β-lactoside as ligands for the Ricinus communis lectins
AUTHOR(S): Fernandex, Paloma; Jimenez-Barbero, Jesus; Martin-Lomas, Manuel
CORPORATE SOURCE: Inst. Quim. Org., CSIC, Madrid, 28006, Spain
SOURCE: Carbohydrate Research (1994), 254, 61-79
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:36028

AB The synthesis of all the possible monomethyl ethers of Me β-lactoside (I) has been performed from I in a straightforward way, making use of the different reactivity of the hydroxyl groups in alkylation and stannylation reactions. In addition, the deoxyfluoro derivs. of I at positions, 6, 3', 4', epi-4', and 6' have been prepared by rea tin of te appropriate substrates with diethylaminosulfur trifluoride or tetrabutylammonium fluoride. Finally, the 6-deoxyiodo and 6'-bormodeoxy analogs of I have also been prepared

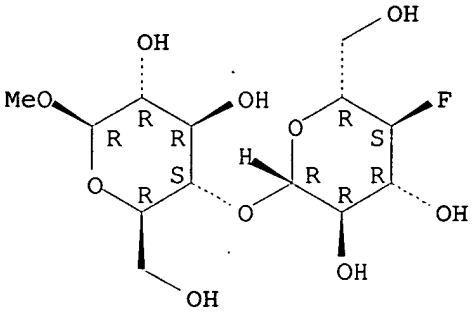
IT 149457-67-0P 155590-30-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 149457-67-0 HCAPLUS
CN β-D-Glucopyranoside, methyl 4-O-(4-deoxy-4-fluoro-β-D-galactopyranosyl)- (CA INDEX NAME)

Absolute stereochemistry.



RN 155590-30-0 HCAPLUS
CN β-D-Glucopyranoside, methyl 4-O-(4-deoxy-4-fluoro-β-D-glucopyranosyl)- (CA INDEX NAME)

Absolute stereochemistry.

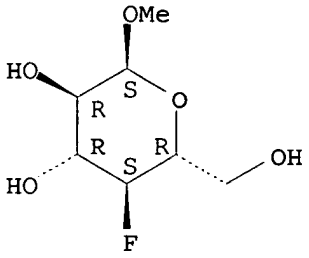


L24 ANSWER 33 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:436000 HCAPLUS
DOCUMENT NUMBER: 121:36000
TITLE: Conformational Analysis. Part 20 Conformational analysis of 4-deoxy-4-fluoro-D-glucose and 6-deoxy-6-fluoro-D-galactose in solution
AUTHOR(S): Abraham, Raymond J.; Chambers, Eric J.; Thomas, W. Anthony
CORPORATE SOURCE: Dep. Chem., Univ. Liverpool, Liverpool, L69 3BX, UK
SOURCE: Magnetic Resonance in Chemistry (1994), 32(4), 248-54
CODEN: MRCHEG; ISSN: 0749-1581
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The 1H and 19F NMR spectra of the α- and β-pyranose anomers of 4-deoxy-4-fluoro-D-glucose (4FG) and 6-deoxy-6-fluoro-D-galactose (6FGA) in methanol-d4, DMSO-d6, acetone-d6 and D2O solution are reported. Computer anal. of the ABMX spectra of the CH-CH2F fragments gives accurate vicinal HH and HF coupling consts. An iterative computational anal. of the observed vicinal couplings in this fragment for 6FG, 6FGA and other mols. allows the determination of both the individual rotamer couplings and the rotamer populations. Consideration of the derived rotamer couplings strongly suggests that the correct assignment for the prochiral C-6 methylene protons in 6FG is that with the 6S proton having the larger coupling to H-5. This is the reverse of the assignment of these protons in D-glucose. In contrast, the assignment of these protons in 6FGA follows that given previously for D-galactose. The relative energies for the conformations about the C-5-C-6 bond for 4FG, 6FG and 6FGA are given from the derived rotamer populations. For 6FGA the rotamer in which the fluorine is antiperiplanar to C-4 is particularly favored. For 4FG the rotamer with OH anti-periplanaer to the ring O is highly unfavored, but the other two rotamers are of almost equal energy. Consideration of the effect of replacing hydroxyl by fluorine in these mols. indicates that any hydrogen bonding involving the C-4 or C-6 hydroxyls plays little part in determining the conformer energies of glucose or galactose in polar solns.

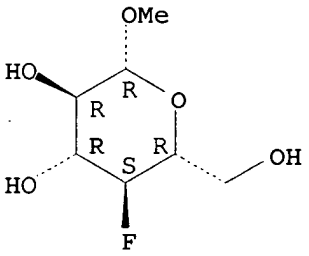
IT 56926-53-5 141990-24-1
RL: PROC (Process)
(conformational anal. of)
RN 56926-53-5 HCAPLUS
CN α-D-Glucopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



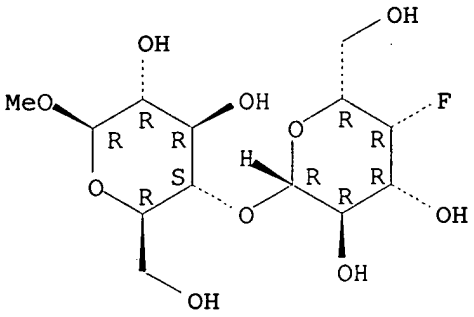
RN 141990-24-1 HCAPLUS
CN β-D-Glucopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



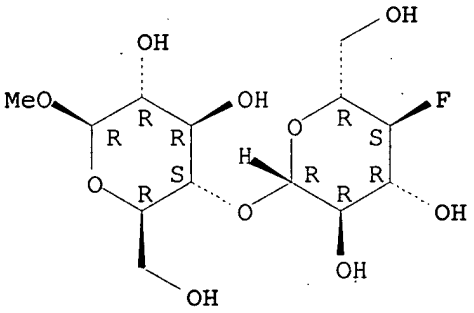
L24 ANSWER 34 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:409842 HCAPLUS
DOCUMENT NUMBER: 121:9842
TITLE: The conformation of some halodeoxy analogs of methyl β-lactoside in D2O and DMSO-d6 solutions
AUTHOR(S): Fernandez, Paloma; Jimenez-Barbero, Jesus
CORPORATE SOURCE: Grupo de Carbohidratos, Inst. de Quim. Org. Gen., Madrid, 28006, Spain
SOURCE: Journal of Carbohydrate Chemistry (1994), 13(2), 207-33
CODEN: JCACDM; ISSN: 0732-8303
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The solution conformation of several halodeoxy analogs of Me β-lactoside has been analyzed using mol. mechanics and dynamics calcns. and NMR data (variable temperature and NOE expts.).
IT 149457-67-0 155590-30-0
RL: PRP (Properties)
(conformation of)
RN 149457-67-0 HCAPLUS
CN β-D-Glucopyranoside, methyl 4-O-(4-deoxy-4-fluoro-β-D-galactopyranosyl)- (CA INDEX NAME)

Absolute stereochemistry.



RN 155590-30-0 HCAPLUS
CN β-D-Glucopyranoside, methyl 4-O-(4-deoxy-4-fluoro-β-D-glucopyranosyl)- (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 35 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1993:510916 HCAPLUS
DOCUMENT NUMBER: 119:110916
TITLE: Hydrogen-bonding pattern of methyl β-lactoside binding to the Ricinus communis lectins
AUTHOR(S): Solis, Dolores; Fernandez, Paloma; Diaz-Maurino, Teresa; Jimenez-Barbero, Jesus; Martin-Lomas, Manuel
CORPORATE SOURCE: Inst. Quim. Fis. "Rocasolano", CSIC, Madrid, Spain
SOURCE: European Journal of Biochemistry (1993), 214(3), 677-83
CODEN: EJBCAI; ISSN: 0014-2956
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The binding of O-Me and fluorodeoxy derivs. of Me β-lactoside to the R. communis toxin (RCA60) and agglutinin (RCA120) was studied in order to determine the donor/acceptor relationships of the hydrogen bonds between the hydroxyl groups of Me β-lactoside and the binding sites of the lectins. Free energy contributions of the hydrogen bonds at each position have been estimated from these data and from those previously reported for the monodeoxy derivs.. The nature of the groups of the lectins involved in hydrogen bonding has been predicted on the basis of the free energy data. Anal. of the results indicates that both the C-3' and C-4' hydroxyl groups act as hydrogen-bond donors to charged groups of both RCA60 and RCA120. The C-6' and probably also the C-2' hydroxyl groups participate both as donors and as acceptors of two hydrogen bonds with neutral groups of the lectins. The C-6 hydroxyl group possibly acts as a donor of a weak hydrogen bond to a neutral group in RCA60, but not in RCA120. The results provide a mol. basis to explain some features of the binding specificity of the lectins. Comparison of RCA60 binding data with the recently refined X-ray crystal structure of the RCA60-lactose complex shows

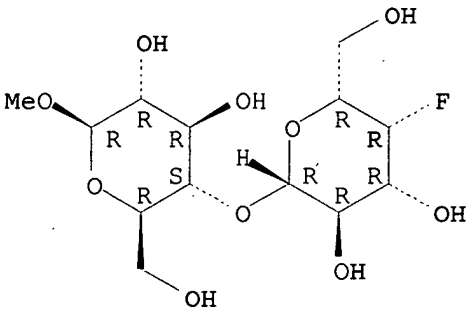
similarities but also some discrepancies that can be attributed to the marked influence of the pH on the carbohydrate-lectin interaction.

IT 149457-67-0
RL: BIOL (Biological study)
(Me lactoside derivs. binding to lectins of Ricinus communis in relation to)

RN 149457-67-0 HCAPLUS

CN β-D-Glucopyranoside, methyl 4-O-(4-deoxy-4-fluoro-β-D-galactopyranosyl)- (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 36 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:607845 HCAPLUS

DOCUMENT NUMBER: 117:207845

TITLE: Binding energy and catalysis. Fluorinated and deoxygenated glycosides as mechanistic probes of Escherichia coli (lacZ) β-galactosidase

AUTHOR(S): McCarter, John D.; Adam, Michael J.; Withers, Stephen G.

CORPORATE SOURCE: Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.

SOURCE: Biochemical Journal (1992), 286(3), 721-7
CODEN: BIJOAK; ISSN: 0306-3275

DOCUMENT TYPE: Journal

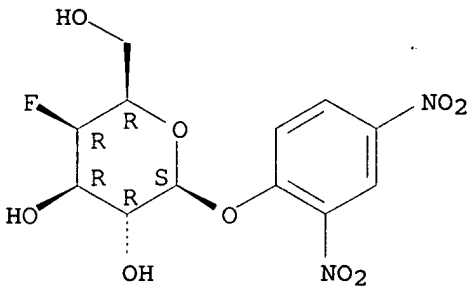
LANGUAGE: English

AB Kinetics parameters for the hydrolysis of a series of deoxy and deoxyfluoro analogs of 2',4'-dinitrophenyl β-D-galactopyranoside by E. coli (lacZ) β-galactosidase have been determined and rates found to be two to nine orders of magnitude lower than that for the parent compound These large rate redns. result primarily from the loss of transition-state binding interactions due to the replacement of sugar hydroxy groups, and such interactions are estimated to contribute at least 16.7 kJ (4 kcal)·mol-1 to binding at the 3, 4 and 6 positions and more than 33.5 kJ (8 kcal)·mol-1 at the 2 position. The existence of a linear free-energy relationship between log(kcat./Km) for these compds. and the logarithm of the first-order rate constant for their spontaneous hydrolysis demonstrates that electronic effects are also important and provides direct evidence for oxocarbonium ion character in the enzymic transition state. A covalent intermediate which turns over only extremely slowly (t1/2 = 45 h) accumulates during hydrolysis of the 2-deoxyfluorogalactoside, and kinetic parameters for its formation have been determined This intermediate is nonetheless catalytically competent, since it re-activated much more rapidly in the presence of the transglycosylation acceptors methanol or glucose, thereby providing support for the notion of a covalent intermediate during hydrolysis of the parent substrates.

IT 144220-98-4
RL: RCT (Reactant); RACT (Reactant or reagent)

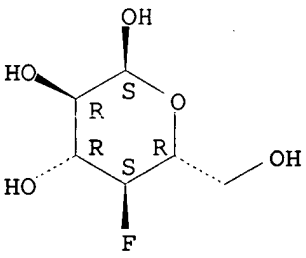
(reaction of, with galactosidase of Escherichia coli, kinetics of)
RN 144220-98-4 HCAPLUS
CN β-D-Galactopyranoside, 2,4-dinitrophenyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



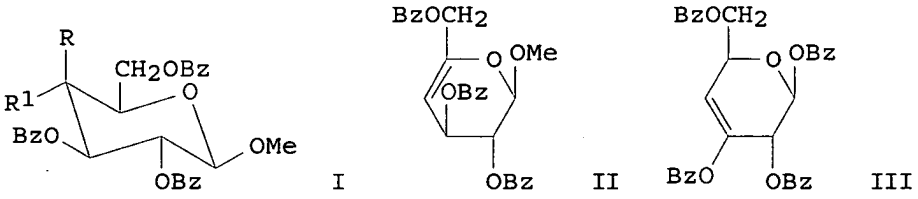
L24 ANSWER 37 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:551218 HCAPLUS
DOCUMENT NUMBER: 117:151218
TITLE: Conformational analysis of 6-deoxy-6-fluoro-D-glucopyranose, 6-deoxy-6-fluoro-D-galactopyranose, and 4-deoxy-4-fluoro-D-glucopyranose in solution by proton NMR spectroscopy
AUTHOR(S): Abraham, Raymond J.; Chambers, Eric J.; Thomas, W. Anthony
CORPORATE SOURCE: Sch. Chem., Univ. Liverpool, Liverpool, L69 3BX, UK
SOURCE: Carbohydrate Research (1992), 226(1), C1-C5
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The C5-C6 rotamer populations of title compds. based on 1H NMR spectra in D2O and either CD3CDCD3 or DMSO-D6, are reported.
IT 62182-11-0
RL: PRP (Properties)
(conformation of, NMR in relation to)
RN 62182-11-0 HCAPLUS
CN α-D-Glucopyranose, 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



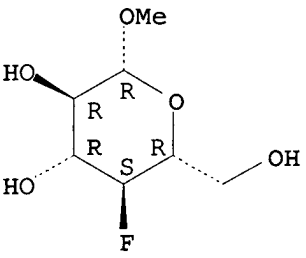
L24 ANSWER 38 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:449057 HCAPLUS
DOCUMENT NUMBER: 117:49057
TITLE: Two methyl tri-O-benzoylhexenopyranosides are amongst the products of the reaction of methyl 2,3,6-tri-O-benzoyl-β-D-galactopyranoside with DAST

AUTHOR(S): Petrakova, Eva; Yeh, Herman J. C.; Kovac, Pavol; Glaudemans, Cornelis P. J.
CORPORATE SOURCE: NIDDK, Natl. Inst. Health, Bethesda, MD, 20892, USA
SOURCE: Journal of Carbohydrate Chemistry (1992), 11(3), 407-12
CODEN: JCACDM; ISSN: 0732-8303
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:49057
GI



AB The reaction of galactopyranoside I (R = OH, R1 = H) with DAST gave the fluoroglucopyranoside I (R = H, R1 = F) and two elimination products II and III.
IT 141990-24-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 141990-24-1 HCAPLUS
CN β-D-Glucopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 39 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:36841 HCAPLUS
DOCUMENT NUMBER: 116:36841
TITLE: Binding energy and catalysis: deoxyfluoro sugars as probes of hydrogen bonding in phosphoglucomutase
AUTHOR(S): Percival, M. David; Withers, Stephen G.
CORPORATE SOURCE: Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.
SOURCE: Biochemistry (1992), 31(2), 498-505
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Ests. of the contributions of H-bonding interactions in rabbit muscle phosphoglucomutase with each of the sugar OH groups to the binding of the substrate, α-D-glucopyranosyl phosphate, both in the ground state and at the transition state for the initial phosphoryl transfer, were obtained by kinetic studies. Michaelis parameters (kcat and Km) for a complete series of deoxy- and deoxyfluoro-α-D-glucopyranosyl

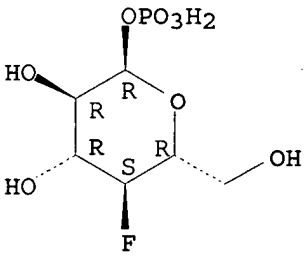
phosphates provided insight into specific interactions with each OH group at the transition state. The Ki values for a series of deoxygenated and fluorinated analogs of the competitive inhibitor, 6-deoxy-6-fluoro-α-D-glucopyranosyl phosphate, provided insight into ground-state interactions. Interactions at each OH group were found to strengthen only slightly upon progressing from the ground state to the transition state in contrast to that seen with glycogen phosphorylase where transition-state interactions became much stronger. This was in accord with the mechanisms for these 2 enzymes where no distortion of the sugar ring occurs for phosphoglucomutase, whereas considerable distortion is expected for glycogen phosphorylase.

IT 109923-28-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phosphoglucomutase of muscle, kinetics of)

RN 109923-28-6 HCAPLUS

CN α-D-Glucopyranose, 4-deoxy-4-fluoro-, 1-(dihydrogen phosphate) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 40 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:36840 HCAPLUS

DOCUMENT NUMBER: 116:36840

TITLE: Fluorine-19 NMR investigations of the catalytic mechanism of phosphoglucomutase using fluorinated substrates and inhibitors

AUTHOR(S): Percival, M. David; Withers, Stephen G.

CORPORATE SOURCE: Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.

SOURCE: Biochemistry (1992), 31(2), 505-12
CODEN: BICHAW; ISSN: 0006-2960

DOCUMENT TYPE: Journal

LANGUAGE: English

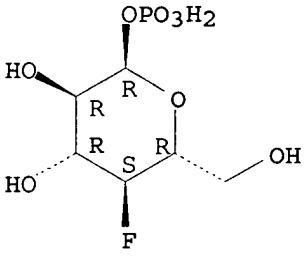
AB The complexes of rabbit muscle phosphoglucomutase with a number of fluorinated substrate analogs were investigated by 19F NMR and the effects of the binding of Li+ and Cd2+ to these complexes were determined Very large downfield chemical shift changes (-14 to -19 ppm) accompanied the binding of the inhibitors, 6-deoxy-6-fluoro-α-D-glucopyranosyl phosphate and α-glucosyl fluoride 6-phosphate, to the phosphoenzyme. Smaller shift changes were observed for ligands substituted with F at other positions. The addition of Li+ to enzyme/fluorinated ligand complexes caused a 102- to 103-fold decrease in ligand dissociation consts. as witnessed by the change from intermediate to slow-exchange conditions in the NMR spectra. Measurement of the 19F NMR spectra of complexes of the Li+-enzyme with each of the fluoroglucose 1-phosphates and 6-phosphates provided some insight into the environment of each of these F atoms (thus, also parent OH groups) in each of the complexes. The results obtained argued strongly against a single sugar-binding mode for the glucose 1- and 6-phosphates. Two enzyme-bound species were detected in the 19F NMR spectra of the complexes formed by reaction of the Cd2+-phosphoenzyme complex with the 2- and 3-fluoroglucose phosphates. These were tentatively assigned as the

fluoroglucose 1,6-bisphosphate species bound in 2 different modes to the dephosphoenzyme. Only 1 bound species was observed in the case of the 4-fluoroglucose phosphates. The results were consistent with an exchange type of mechanism for the enzyme in which there are 2 distinct glucose ring-binding sites.

IT 109923-28-6 137945-68-7 137945-69-8
RL: BIOL (Biological study)
(phosphoglucomutase of muscle binding of, in lithium presence, fluorine-19 NMR study of)

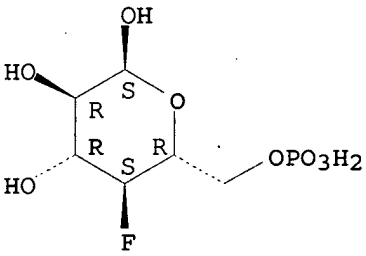
RN 109923-28-6 HCAPLUS
CN α-D-Glucopyranose, 4-deoxy-4-fluoro-, 1-(dihydrogen phosphate) (CA INDEX NAME)

Absolute stereochemistry.



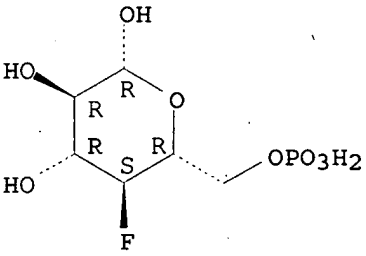
RN 137945-68-7 HCAPLUS
CN α-D-Glucopyranose, 4-deoxy-4-fluoro-, 6-(dihydrogen phosphate) (CA INDEX NAME)

Absolute stereochemistry.



RN 137945-69-8 HCAPLUS
CN β-D-Glucopyranose, 4-deoxy-4-fluoro-, 6-(dihydrogen phosphate) (CA INDEX NAME)

Absolute stereochemistry.



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CA SUBSCRIBER PRICE	0.00	-57.60

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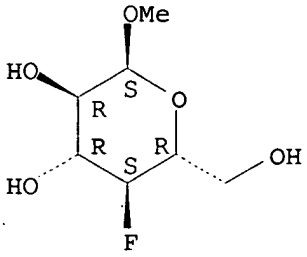
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jan 11, 2008 (20080111/UP).

=> d l24 ibib abs hitstr 41-80
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:y

L24 ANSWER 41 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:22075 HCAPLUS
DOCUMENT NUMBER: 114:22075
TITLE: Binding characteristics of IgA 16.4.12E, a monoclonal antibody with specificity for the nonreducing terminal epitope of α-(1→6)-dextrans. Comparisons between IgA hybridoma 16.4.12E and myeloma W3129
AUTHOR(S): Nashed, Eugenia M.; Perdomo, Guillermo R.; Padlan, Eduardo A.; Kovac, Pavol; Matsuda, Tsukasa; Kabat, Elvin A.; Glaudemans, Cornelis P. J.
CORPORATE SOURCE: Off. Cir., Natl. Inst. Diabetics Dig. Kidney Dis., Bethesda, MD, 20892, USA
SOURCE: Journal of Biological Chemistry (1990), 265(33), 20699-707
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: English
AB IgA 16.4.12E is a murine monoclonal antibody obtained following immunization with isomaltohexose linked to keyhole limpet hemocyanin. Its binding was studied with Me α-D-glucopyranoside and its derivs. bearing deoxy or deoxyfluoro groups, and with the Me α-glycosides of a series of isomalto-oligosaccharides, some bearing deoxy or deoxyfluoro groups at selected positions. The antibody binds optimally to 4 sequential glucopyranosyl residues and that the protein subsite possessing the major affinity binds the terminal, nonreducing glucosyl group of that antigenic epitope. All the hydroxyl groups of that terminal glucosyl group are involved in hydrogen bonding, some in a donating and some in an accepting capacity. The construction of a possible model of the antibody, derived from its known amino acid sequence and the known crystalline structures of two closely related antibodies is described which shows a pronounced cavity in the general Ig combining area which is flanked by 2 solvent-exposed tryptophanyl residues. A model recently reported for antidextran IgA W3129 shows a similar cavity with one such residue. Guided by hydrogen bonds, exptl. deduced from the comparison of the affinities of various derivatized ligands, a speculative fitting is suggested for the nonreducing terminus of the dextran antigen, in the resp. cavities of both IgA 16.4.12E and W3129.
IT 56926-53-5
RL: BIOL (Biological study)
(IgA monoclonal antibody to, binding characteristics and model of)
RN 56926-53-5 HCAPLUS
CN α-D-Glucopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.

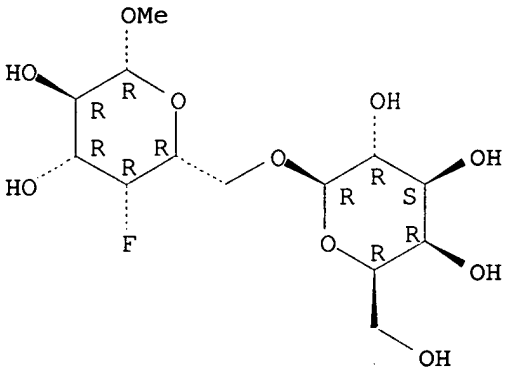


L24 ANSWER 42 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:629180 HCAPLUS
DOCUMENT NUMBER: 113:229180
TITLE: Significant conformational changes in an antigenic carbohydrate epitope upon binding to a monoclonal antibody
AUTHOR(S): Glaudemans, Cornelis P. J.; Lerner, Laura; Daves, G. Doyle, Jr.; Kovac, Pavol; Venable, Richard; Bax, Ad
CORPORATE SOURCE: Dep. Chem., Univ. Wisconsin, Madison, WI, 53706, USA
SOURCE: Biochemistry (1990), 29(49), 10906-11
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Transferred nuclear Overhauser enhancement spectroscopy (TRNOE) was used to observe changes in a ligand's conformation upon binding to its specific antibody. The ligands studied were Me O-β-D-galactopyranosyl(1→6)-β-D-4-deoxy-4-fluorogalactopyranoside (I) and its selectively deuteriated analog Me O-β-D-galactopyranosyl(1→6)-β-D-4-deoxy-2-deuterio-4-fluorogalactopyranoside (II). The monoclonal antibody was mouse IgA X24. The solution conformation of the free ligand II was inferred from measurements of vicinal 1H-1H coupling consts., long-range 1H-13C coupling consts., and NOE cross-peak intensities. For free ligand, both galactosyl residues adopt a regular chair conformation, but the NMR spectra are incompatible with a single unique conformation of the glycosidic linkage. Anal. of 1H-1H and 1H-13C coupling consts. indicates that the major conformer has an extended conformation: .vphi. = -120°; ψ = 180°; and ω = 75°. TRNOE measurements on I and II in the presence of the specific antibody indicate that the pyranose ring pucker of each galactose ring remains unchanged, but rotations about the glycosidic linkage occur upon binding to X24. Computer calcns. indicate that there are two sets of torsion angles that satisfy the observed NMR constraints, namely, .vphi. = -152°; ψ = -128°; and ω = -158°; and a conformer with .vphi. = -53°; ψ = 154°; and ω = -173°. Neither conformation is similar to any of the observed conformations of the free disaccharide. Therefore, the X24 antibody binding alters the conformation of its ligand upon binding. A new method, based on changes in the fluorine longitudinal relaxation rate, is used to measure the ligand-antibody dissociation rate constant At 55°, this rate constant is 100 s-1.

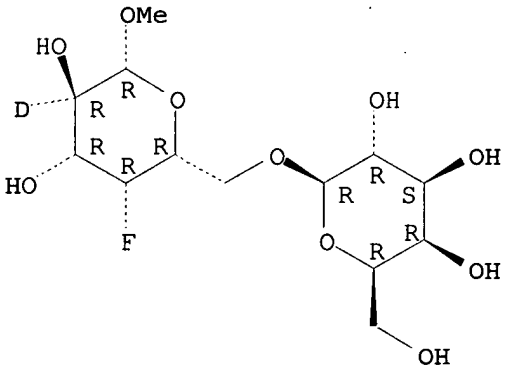
IT 92397-31-4 129707-58-0
RL: BIOL (Biological study)
(of antigen epitope, conformation of, changes in, upon binding to monoclonal antibodies)
RN 92397-31-4 HCAPLUS
CN β-D-Galactopyranoside, methyl 4-deoxy-4-fluoro-6-O-β-D-galactopyranosyl- (CA INDEX NAME)

Absolute stereochemistry.



RN 129707-58-0 HCAPLUS
CN β-D-Galactopyranoside-2-C-d, methyl 4-deoxy-4-fluoro-6-O-β-D-galactopyranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



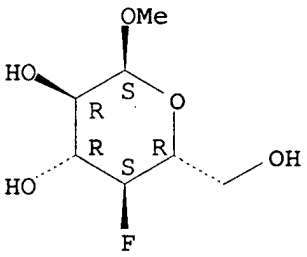
L24 ANSWER 43 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:548627 HCAPLUS
DOCUMENT NUMBER: 113:148627
TITLE: The metabolism of 4-deoxy-4-fluoro-D-glucose in Pseudomonas putida
AUTHOR(S): Sbrissa, Diego; McIntosh, J. M.; Taylor, Norman F.
CORPORATE SOURCE: Dep. Chem. Biochem., Univ. Windsor, Windsor, ON, N9B 3P4, Can.
SOURCE: Carbohydrate Research (1990), 203(2), 271-80
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The synthesis of 4-deoxy-4-fluoro-D-[U-14C]glucose from D-[U-14C]galactose is reported. A 24-h incubation of P. putida with 4-deoxy-4-fluoro-D-[U-14C]glucose gives 95 ± 5% release of fluoride and 4.8 ± 0.2% of the initial radioactivity as 14CO2. After centrifugation, Dowex-1 [borate-2-] column chromatog. of the cell supernatant, which accounts for 52.4 ± 1.3% of the initial radioactivity, allows the isolation of a major radioactive metabolite. By 13C- and 1H-NMR spectroscopy and by mass spectrometric anal., this metabolite is identified as 2,3-dideoxy-D-glyceropentonic acid. Extensive dialysis of the remaining cell pellet, followed by sonication and appropriate centrifugation, allows isolation of a cell envelope fraction with 0.4 ± 0.05% of the initial radioactivity. Gel filtration of this SDS-solubilized fraction shows all the

radioactivity to be in a large mol. weight peptidoglycan-protein complex (>400,000 daltons). Following lysozyme treatment, this complex now elutes from the same column with a lower mol. weight (>14,000 daltons). The radioactivity of the peptidoglycan complex is shown to be due to the presence of aspartate, threonine, and glutamate.

IT 56926-53-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 56926-53-5 HCAPLUS
CN α-D-Glucopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

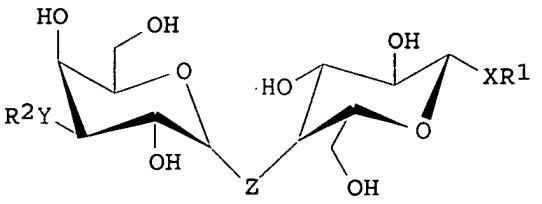
Absolute stereochemistry.



L24 ANSWER 44 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:459768 HCAPLUS
DOCUMENT NUMBER: 113:59768
TITLE: Preparation of galabioside analogs as antibacterials
INVENTOR(S): Magnusson, Hans Goeran; Kihlberg, Jan Olof
PATENT ASSIGNEE(S): Symbicom AB, Swed.
SOURCE: PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
WO 9001488	A1	19900222	WO 1989-DK192		19890811	<--
W: AU, DK, FI, JP, KR, NO, US						
RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE						
IL 91269	A	19941111	IL 1989-91269		19890809	<--
AU 8940749	A	19900305	AU 1989-40749		19890811	<--
AU 634976	B2	19930311				
EP 428605	A1	19910529	EP 1989-909545		19890811	<--
EP 428605	B1	19941019				
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE						
JP 04506509	T	19921112	JP 1989-508951		19890811	<--
CA 1332234	C	19941004	CA 1989-608146		19890811	<--
NO 9100503	A	19910412	NO 1991-503		19910208	<--
NO 176518	B	19950109				
NO 176518	C	19950419				
DK 9100228	A	19910211	DK 1991-228		19910211	<--
FI 93016	B	19941031	FI 1991-653		19910211	<--
FI 93016	C	19950210	FI 1991-653		19910211	<--
US 5474986	A	19951212	US 1991-689077		19910411	<--
PRIORITY APPLN. INFO.:			DK 1988-4550	A	19880812	
			WO 1989-DK192	A	19890811	

OTHER SOURCE(S): MARPAT 113:59768
GI



I

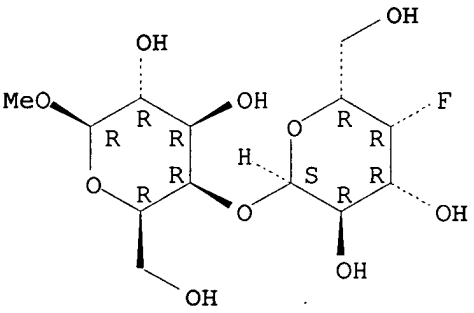
AB The title compds. [I; R1 = alkyl, alkenyl, alkynyl, silylethyl, (substituted) aryl, etc.; R2 = mono- or disaccharide residue connected via glycosidic bond, alkyl, alkenyl, alkynyl, etc.; X = O, S, SO2, CH2, (substituted) amino, etc.; Y = O, (substituted) amino, etc.; Z = O, S, SO2, CH2, useful for treatment and prevention of bacterial infection, were prepared Condensation of Me 2,3,6-tri-O-benzoyl-β-D-galactopyranoside (preparation given) with 2,4,6-tri-O-benzyl-3-O-methyl-D-galactopyranosyl chloride gave, after deprotection, I [R1 = Me, R2 = H, X = Y = Z = O), which at 0.087 mM inhibited 50% of the agglutination of human erythrocytes by Escherichia coli.

IT 122204-34-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as antibacterial)

RN 122204-34-6 HCAPLUS

CN β-D-Galactopyranoside, methyl 4-O-(4-deoxy-4-fluoro-α-D-galactopyranosyl)- (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 45 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:437021 HCAPLUS

DOCUMENT NUMBER: 113:37021

TITLE: Measurement of active-site homology between potato and rabbit muscle α-glucan phosphorylases through use of a linear free energy relationship

AUTHOR(S): Withers, Stephen G.; Rupitz, Karen

CORPORATE SOURCE: Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.

SOURCE: Biochemistry (1990), 29(27), 6405-9
CODEN: BICHAW; ISSN: 0006-2960

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The Michaelis-Menten parameters (Vmax and Km) for turnover of an extensive series of deoxy and deoxyfluoro derivs. of α-D-glucopyranosyl phosphate by the α-glucan phosphorylase from potato tuber have been determined Very large rate redns. are observed as a consequence of each

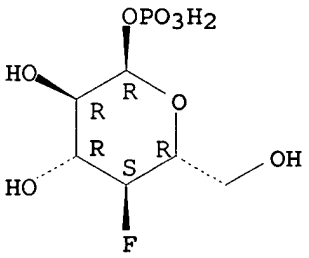
substitution, primarily due to losses in specific binding interactions, most likely H bonding, in the enzymic transition state. Comparison of the Vmax/Km values so determined with those previously measured for rabbit muscle α-glucan phosphorylase reveals an astonishingly similar specificity, especially in light of the phylogenetic separation of their host organisms. This indicates that very similar H-bonding interactions between the enzyme and the substrate must be present at the transition states for the 2 enzymic reactions; therefore, they have very similar active sites. Quantitation of this similarity is achieved by plotting the logarithm of the Vmax/Km value for each substrate analog with the potato enzyme against the same parameter for the muscle enzyme, yielding straight lines (ρ = 0.998 and 0.999) of slope 1.0 and 1.2 for the deoxy and deoxyfluoro substrates, resp. Since the correlation coefficient of such plots is a direct measure of the similarity of the 2 transition-state complexes, thus of the enzyme active sites, it can be used as a measure of active site homol. between the 2 enzymes. The extremely high homol. observed in this case is consistent with the observed sequence homol. at the active site.

IT 109923-28-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with glucan phosphorylase of potato, kinetics of, muscle enzyme active site homol. in relation to)

RN 109923-28-6 HCAPLUS

CN α-D-Glucopyranose, 4-deoxy-4-fluoro-, 1-(dihydrogen phosphate) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 46 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:213437 HCAPLUS

DOCUMENT NUMBER: 112:213437

TITLE: The enzymic synthesis and NMR characterization of specifically deoxygenated and fluorinated glycogens

AUTHOR(S): Withers, Stephen G.

CORPORATE SOURCE: Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.

SOURCE: Carbohydrate Research (1990), 197, 61-73
CODEN: CRBRAT; ISSN: 0008-6215

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The incorporation of several deoxy- and deoxyfluoro-D-glucose analogs into glycogen has been achieved through the action of rabbit muscle glycogen phosphorylase on a number of deoxy- and deoxyfluoro- analogs of α-D-glucopyranosyl phosphate. Time courses for the incorporation of these analogs into glycogen and maltopentaose have been determined, and the introduction of 4-deoxy- or 4-deoxy-4-fluoro-D-glucose units has been demonstrated to terminate after the introduction of 1 sugar unit per non-reducing terminus. Glycogen analogs containing sugars modified at the 3- and 4-positions have been isolated and characterized by 1H-NMR and 19F-NMR spectroscopy, and the extent of incorporation has been confirmed by integration of the new resonances associated with the incorporated residues. Longitudinal (T1) relaxation times have been determined for the two 19F-NMR

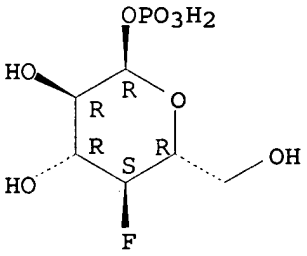
resonances observed for 3-deoxy-3-fluoro-glycogen, and through comparison with the T1 measured for 4-deoxy-4-fluoro-glycogen, the identity (terminal or internal) of each of these 2 resonances was determined Kinetic studies indicate that neither 4-deoxy- nor 4-deoxy-4-fluoro-glycogen can serve as a substrate for glycogen phosphorylase in the direction of glycogen synthesis, proving that these glycogen analogs have been fully substituted. Both of these 4-substituted glycogens are good inhibitors of glycogen phosphorylase.

IT 109923-28-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with glycogen)

RN 109923-28-6 HCAPLUS

CN α-D-Glucopyranose, 4-deoxy-4-fluoro-, 1-(dihydrogen phosphate) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 47 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1989:532049 HCAPLUS

DOCUMENT NUMBER: 111:132049

TITLE: The subsites of monoclonal antidextran IgA W3129

AUTHOR(S): Glaudemans, Cornelis P. J.; Kovac, Pavol; Rao, Arepalli S.

CORPORATE SOURCE: Natl. Inst. Diabetes Dig. Kidney Dis., Natl. Inst. Health, Bethesda, MD, 20892, USA

SOURCE: Carbohydrate Research (1989), 190(2), 267-77
CODEN: CRBRAT; ISSN: 0008-6215

DOCUMENT TYPE: Journal

LANGUAGE: English

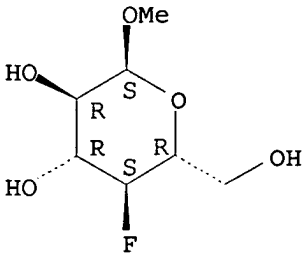
AB Synthetic deoxyfluoro derivs. of Me α-D-glucopyranoside, as well as Me α-glycosides of isomalto-oligosaccharides, some having fluorine substituted for hydroxyl groups at selected positions, were evaluated for their binding with a myeloma monoclonal IgA known to bind only to an oligosaccharide sequence at the nonreducing end of α-(1→6)-linked D-glucopyranans (dextrans). The results are compatible with the antibody's possessing one subsite of high affinity for its D-glucosyl group, the remaining 3 subsites having low affinities for their resp. D-glucosyl residues. The high-affinity antibody-subsite occurs at the interior end of the sequence of 4 subsites, appears to be relatively accessible, and binds the (terminal) nonreducing D-glucosyl group of the oligosaccharidic determinant using 2, and possibly 3, hydroxyl groups in hydrogen bonding.

IT 56926-53-5
RL: BIOL (Biological study)
(monoclonal anti-dextran IgA binding to, high-affinity subsites in)

RN 56926-53-5 HCAPLUS

CN α-D-Glucopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 48 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:515704 HCAPLUS
DOCUMENT NUMBER: 111:115704
TITLE: Preparation of 3-Demethylmevalonic acid derivatives as anticholesteremics and their intermediates
INVENTOR(S): Bergmann, Andreas; Bartmann, Wilhelm; Beck, Gerhard; Lau, Hans Germann
PATENT ASSIGNEE(S): Hoechst A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 30 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3722809	A1	19890119	DE 1987-3722809	19870710 <--
FI 8803250	A	19890111	FI 1988-3250	19880707 <--
EP 302253	A1	19890208	EP 1988-110834	19880707 <--
EP 302253	B1	19930407		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AT 87916	T	19930415	AT 1988-110834	19880707 <--
ES 2054738	T3	19940816	ES 1988-110834	19880707 <--
DK 8803833	A	19890111	DK 1988-3833	19880708 <--
NO 8803074	A	19890111	NO 1988-3074	19880708 <--
NO 172537	B	19930426		
NO 172537	C	19930804		
AU 8818883	A	19890112	AU 1988-18883	19880708 <--
AU 612665	B2	19910718		
JP 01038086	A	19890208	JP 1988-169164	19880708 <--
ZA 8804922	A	19890222	ZA 1988-4922	19880708 <--
US 4898868	A	19900206	US 1988-216752	19880708 <--
HU 51221	A2	19900428	HU 1988-3595	19880708 <--
HU 205071	B	19920330		
CA 1319363	C	19930622	CA 1988-571559	19880708 <--
IL 87037	A	19950330	IL 1988-87037	19880708 <--

PRIORITY APPLN. INFO.: DE 1987-3722809 A 19870710
EP 1988-110834 A 19880707
OTHER SOURCE(S): CASREACT 111:115704; MARPAT 111:115704
GI For diagram(s), see printed CA Issue.
AB The title compds. [I, II; R = (substituted) Ph; X = O, S; Y = CH2; or XY = CH:CH, CH2CH2], useful as anticholesteremics, are prepared, e.g., via reaction of RXH with pyranylmethyl iodides III [R 19 = iodo; R20 = protecting group; R21 = easily hydrolyzable group], oxidation of the resulting III (R19 = RX; R20, R21 as defined above), deprotection, and optional conversion of the resulting I into II or their salts. III (R19 = iodo, R20 = Me3CSiPh2O, R21 = Me) was treated with 2,3,5-(HS)Cl2C6H2CH(C6H4F-p)2 in Me2SO containing K2CO3 at 50° for 6 h to give, after deprotection, I [R = 2-[bis(p-fluorophenyl)methyl]-4,6-dichlorophenyl, X = S, Y = CH2] (IV). In a study using an enzyme preparation

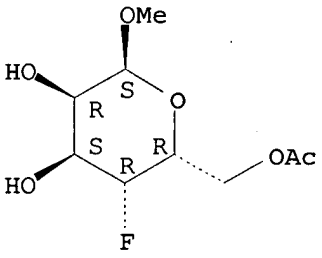
of rat liver microsomes, IV showed an IC50 of 2 + 10-6 M in inhibiting the activity of HMG-CoA reductase.

IT 122451-85-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of anticholesteremics)

RN 122451-85-8 HCAPLUS

CN α-D-Gulopyranoside, methyl 4-deoxy-4-fluoro-, 6-acetate (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 49 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1989:515686 HCAPLUS

DOCUMENT NUMBER: 111:115686

TITLE: Synthetic receptor analogs. 4. Preparation and calculated conformations of the 2'-, 3'-, 4'-, and 6'-deoxy, 3'-O-methyl, 4'-epi, and 4'- and 6'-deoxyfluoro derivatives of methyl 4-O-α-D-galactopyransoyl-β-D-galactopyranoside (methyl β-D-galabioside)

AUTHOR(S): Kihlberg, Jan; Frejd, Torbjoern; Jansson, Karl; Kitzing, Susanna; Magnusson, Goeran

CORPORATE SOURCE: Chem. Cent., Lund Inst. Technol., Lund, S-221 00, Swed.

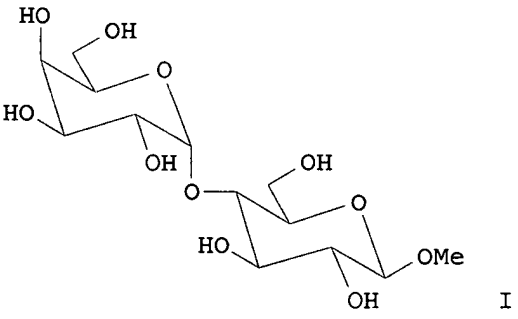
SOURCE: Carbohydrate Research (1989), 185(2), 171-90
CODEN: CRBRAT; ISSN: 0008-6215

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 111:115686

GI



I

AB The glycosyl chlorides of the 3-O-Me and 4-deoxy-4-fluoro O-benzylated derivs. of D-galactopyranose and 2,3,4,6-tetra-O-benzyl-D-glucopyranose were condensed with Me 2,3,6-tri-O-benzoyl-β-D-galactopyranoside to give, after deprotonation, the 3'-O-Me, 4'-deoxy-4'-fluoro, and 4'-epi

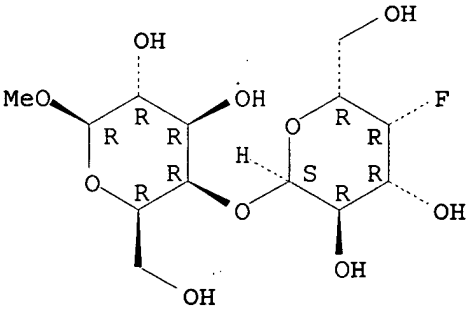
derivs., resp., of Me β-D-galabioside (I). The glycosyl fluorides of 2,3,4-tri-O-benzyl-D-fucopyranose and the 3-deoxy- and 4-deoxy-O-benzylated derivs. of D-galactopyranose were condensed with Me 2,3,6-tri-O-benzyl-β-D-galactopyranoside II, to give, after deprotection, the 6'-deoxy, 3'-deoxy, and 4'-deoxy derivs. of I, resp. The 2'-deoxy derivative of I was prepared by N-iodosuccinimide-induced condensation of 3,4,6-tri-O-acetyl-D-galactal and II followed by deprotection. Treatment of Me 2,3,6-tri-O-benzyl-4-O-(2,3-di-O-benzoyl-α-D-galactopyranosyl)-β-D-galactopyranoside with Et2NSF3 (DAST), followed by deprotection, provided the 6'-deoxy-6'-fluoro derivative of I. Mol. mechanics calcns. yielded conformations for the title compds. with small deviations from the calculated conformation for I.

IT 122204-34-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and calculated conformation of)

RN 122204-34-6 HCAPLUS

CN β-D-Galactopyranoside, methyl 4-O-(4-deoxy-4-fluoro-α-D-galactopyranosyl)- (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 50 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1989:91168 HCAPLUS

DOCUMENT NUMBER: 110:91168

TITLE: Fluorinated and deoxygenated substrates as probes of transition state structure in glycogen phosphorylase

AUTHOR(S): Street, Ian P.; Rupitz, Karen; Withers, Stephen G.

CORPORATE SOURCE: Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.

SOURCE: Biochemistry (1989), 28(4), 1581-7
CODEN: BICHAW; ISSN: 0006-2960

DOCUMENT TYPE: Journal

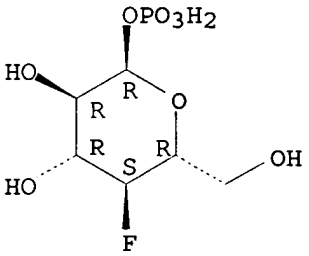
LANGUAGE: English

AB A series of deoxyfluoro- and deoxy-α-D-glucopyranosyl phosphates were tested as substrates of rabbit muscle glycogen phosphorylase b. All were found to be utilized by the enzyme, but at substantially reduced rates. Values of Vmax/Km for these analogs were 102-105-fold lower than that for the parent substrate. The large rate redns. were suggested to arise from a combination of intrinsic electronic effects and poorer binding of these substrates at the transition state. The data provided substantial evidence for an oxocarbonium-ion-like transition state. They also provided ests. of the strengths of H-bonds to individual sugar OH groups at the transition state of the reaction. Further, comparison of such data with those obtained for glucose analogs binding as inhibitors to T-state phosphorylase suggested that these 2 glucose subsites are essentially identical; thus, the glucose pocket remains intact during the conformational transition associated with activation of the enzyme.

IT 109923-28-6
RL: RCT (Reactant); RACT (Reactant or reagent)

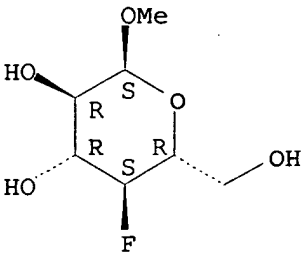
(reaction of, with phosphorylase b, kinetics of, enzyme transition state structure in relation to)
RN 109923-28-6 HCAPLUS
CN α-D-Glucopyranose, 4-deoxy-4-fluoro-, 1-(dihydrogen phosphate) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 51 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1988:438089 HCAPLUS
DOCUMENT NUMBER: 109:38089
TITLE: Synthesis and NMR spectra of methyl 2-deoxy-2-fluoro- and 3-deoxy-3-fluoro-α- and β-D-glucopyranosides
AUTHOR(S): Kovac, Pavol; Yeh, Herman J. C.; Glaudemans, P. J.
CORPORATE SOURCE: NIDDK, Natl. Inst. Health, Bethesda, MD, 20892, USA
SOURCE: Carbohydrate Research (1987), 169, 23-34
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:38089
AB Me 3-deoxy-3-fluoro-α- and β-D-glucopyranosides and α- and β-D-glucofuranosides were prepared by methanolysis of 3-deoxy-3-fluoro-1,2:5,6-di-O-isopropylidene-α-D-glucofuranose. Crystalline 3,4,6-tri-O-acetyl-2-deoxy-2-fluoro-α-D-glucopyranosyl chloride (I) and bromide were prepared from 1,3,4,6-tetra-O-acetyl-2-deoxy-2-fluoro-β-D-glucopyranose (II). Reaction of I with MeOH under the conditions of both silver triflate- and silver perchlorate-catalyzed glycosylation showed remarkable lack of stereoselectivity for the α-glycoside, despite the presence at C-2 of the F presumably not capable of neighboring-group participation. Pure Me 2-deoxy-2-fluoro-α- and β-D-glucopyranosides were obtained by fractional crystallization from the mixture formed by methanolysis of II. The structure of these substances as well as of several other derivs. of 2-deoxy-2-fluoro- and 3-deoxy-3-fluoro-D-glucose were verified by (1H, 13C, and 19F) NMR.
IT 56926-53-5P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and NMR of)
RN 56926-53-5 HCAPLUS
CN α-D-Glucopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 52 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1988:35526 HCAPLUS
DOCUMENT NUMBER: 108:35526
TITLE: The role of C-4-substituted mannose analogs in protein glycosylation. Effect of the guanosine diphosphate esters of 4-deoxy-4-fluoro-D-mannose and 4-deoxy-D-mannose on lipid-linked oligosaccharide assembly
AUTHOR(S): McDowell, William; Grier, Thomas J.; Rasmussen, James R.; Schwarz, Ralph T.
CORPORATE SOURCE: Inst. Virol., Justus Liebig Univ., Giessen, 6300, Fed. Rep. Ger.
SOURCE: Biochemical Journal (1987), 248(2), 523-31
CODEN: BIJOAK; ISSN: 0306-3275
DOCUMENT TYPE: Journal
LANGUAGE: English

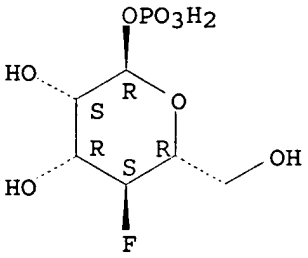
AB The effects of the GDP esters of 4-deoxy-4-fluoro-D-mannose (GDP-4FMan) and 4-deoxy-D-mannose (GDP-4dMan) on reactions of the dolichol pathway were investigated by studies with chick embryo cell microsomal membranes in vitro and in BHK cells in vivo. Each nucleotide sugar analog inhibited lipid-linked oligosaccharide biosynthesis in a concentration-dependent manner. GDP-4FMan blocked in vitro the addition of mannose to Dol-PP-(GlcNAc)2Man from GDP-Man (where Dol represents dolichol and P is a phosphate group), but did not interfere with the formation of Dol-P-Man, Dol-P-Glc (where Glc = glucose), and Dol-PP-(GlcNAc)2. Although GDP-4FMan and Dol-P-4FMan were identified as metabolites of 4FMan in BHK cells labeled with [1-14C]4FMan, GDP-4FMan was a very poor substrate for GDP-Man:Dol-P mannosyltransferase and Dol-P-4FMan could only be synthesized in vitro if the chick embryo cell membranes were primed with Dol-P. Therefore, the inhibition of lipid-linked oligosaccharide formation in BHK cells treated with 4FMan (Grier, T.J.; Rasmussen, J.R., 1984) appears to be due primarily to a blockage in the formation of Dol-PP-(GlcNAc)2Man2 by GDP-4FMan. In contrast, GDP-4dMan was a substrate for those mannosyltransferases that catalyze the transfer of the 1st 5 mannose residues to Dol-PP-(GlcNAc)2. In addition, GDP-4dMan was a substrate for GDP-Man:Dol-P mannosyltransferase, which catalyzed the formation of Dol-P-4dMan. As a consequence of this, the formation of Dol-P-Man, Dol-P-Glc, and Dol-PP-(GlcNAc)2 may be inhibited through competition for Dol-P. In BHK cells treated with 10 mM 4dMan, Dol-PP-(GlcNAc)2Man9 was the major lipid-linked oligosaccharide detected. Nearly normal extents of protein glycosylation were observed, but very little processing to complex oligosaccharides occurred, and the high-mannose structures were smaller than those in untreated cells.

IT 112143-28-9
RL: FORM (Formation, nonpreparative)
(formation of, by animal cells and microsomes)
RN 112143-28-9 HCAPLUS
CN α-D-Mannopyranose, 4-deoxy-4-fluoro-, 1-ester with dolichol dihydrogen phosphate (9CI) (CA INDEX NAME)

CM 1

CRN 270076-20-5
CMF C6 H12 F O8 P

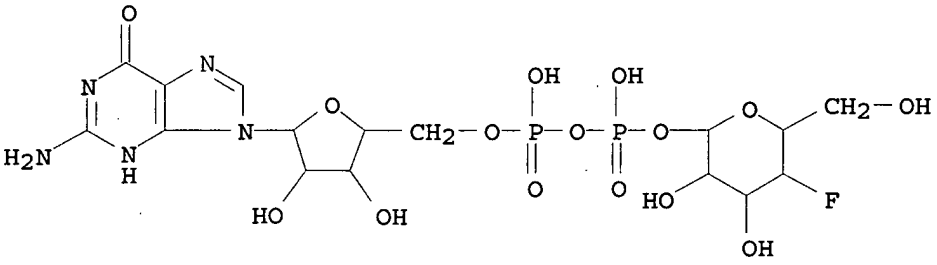
Absolute stereochemistry.



CM 2

CRN 11029-02-0
CMF Unspecified
CCI MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
IT 112028-38-3
RL: BIOL (Biological study)
(lipid-linked oligosaccharide formation by animal cells and microsomes response to)
RN 112028-38-3 HCAPLUS
CN Guanosine 5'-(trihydrogen diphosphate), P'-(4-deoxy-4-fluoro-α-D-mannopyranosyl) ester (9CI) (CA INDEX NAME)



L24 ANSWER 53 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1987:631696 HCAPLUS
DOCUMENT NUMBER: 107:231696
TITLE: Thermodynamic analysis of inducer binding to the lactose repressor protein: contributions of galactosyl hydroxyl groups and β-substituents
AUTHOR(S): Chakerian, Artemis E.; Olson, John S.; Matthews, Kathleen Shive
CORPORATE SOURCE: Dep. Biochem., Rice Univ., Houston, TX, 77251, USA
SOURCE: Biochemistry (1987), 26(23), 7250-5
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Kinetic and equilibrium studies of the binding of modified β-D-galactoside sugars to the lac repressor were carried out to generate thermodn. data for protein-inducer interactions. The energetic contributions of the galactosyl hydroxyl groups to binding were assessed using a series of Me

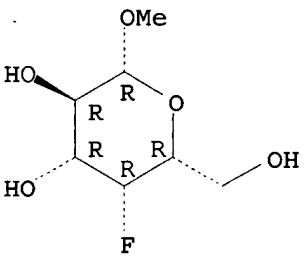
deoxyfluoro-β-D-galactosides. The C-3 and C-6 OH groups contributed ≤-2.3 and -1.7 kcal/mol to the binding free energy change, resp., whereas the C-4 OH group provided only a nominal contribution (-0.1 kcal/mol). Favorable contributions to the total binding free energy change were observed for replacement of O-Me by S-Me at the β-anomeric position and for S-Me by S-iso-Pr. Neg. ΔH° (enthalpy) values characteristic of protein-sugar complexes were observed for a series of β-D-galactosides differing at the β-glycosidic position. A decrease in ΔH° of .apprx.6 kcal/mol upon replacement of the O-Me substituent by S-Me indicates a substantial increase in van der Waals' interactions and(or) H bonding in this region of the ligand binding site. The more favorable free energy change for the binding of the S-iso-Pr vs. S-Me compound is due mainly to more pos. entropic contributions, consistent with an increase in apolar interactions. Thermodn. parameters for iso-Pr β-D-thiogalactoside (IPTG) binding at neutral pH are in agreement with previously published results. Arrhenius plots of kinetic rate consts. for the binding of IPTG, Me β-D-galactoside, and Me β-D-thiogalactoside to the repressor revealed a protein structural transition at 12°. All of the exptl. data are consistent with the hypothetical sugar binding site for repressor protein proposed by C. F. Sams et al. (1984).

IT 51385-54-7
RL: BIOL (Biological study)
(lactose repressor binding of, kinetics and thermodn. of)

RN 51385-54-7 HCAPLUS

CN β-D-Galactopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 54 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1987:496978 HCAPLUS

DOCUMENT NUMBER: 107:96978

TITLE: The synthesis and hydrolysis of a series of deoxyfluoro-D-glucopyranosyl phosphates

AUTHOR(S): Withers, Stephen G.; MacLennan, David J.; Street, Ian P.

CORPORATE SOURCE: Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.

SOURCE: Carbohydrate Research (1986), 154, 127-44
CODEN: CRBRAT; ISSN: 0008-6215

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 107:96978

AB The synthesis of all 4 deoxyfluoro-α-D-glucopyranosyl phosphates is described. For example, 1,2,3,4-tetra-O-acetyl-β-D-glucopyranose was treated with diethylaminosulfur trifluoride in CH2Cl2 in the presence of 2,4,6-trimethylpyridine to give 68% 1,2,3,4-tetra-O-acetyl-6-deoxy-6-fluoro-β-D-glucopyranose, which was heated with H3PO4 and then treated with cyclohexylamine in H2O to give 70% 6-deoxy-6-fluoro-α-D-glucopyranosyl bis(cyclohexylammonium) phosphate. Rate consts. for their acid-catalyzed hydrolysis were determined, and fluorine substitution was shown

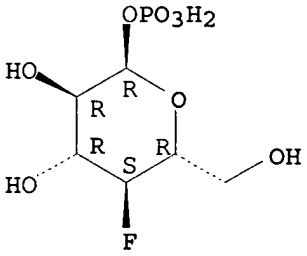
to have a significant effect in lowering the rate, particularly when the substitution is adjacent to the anomeric center. The hydrolysis of 2-deoxy-2-fluoro-α-D-glucopyranosyl phosphate was studied in more detail, and an activation entropy and enthalpy were determined for hydrolysis in M HClO4 at 60°. The pH dependence of its hydrolysis was investigated, and rate consts. for hydrolysis of the monoanion and neutral species were extracted Hydrolysis of the monoanion is not significantly affected by fluorine substitution, as expected. The ability or inability of several mechanistically distinct enzymes to utilize these fluorinated substrates is rationalized in the light of these findings.

IT 109923-29-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acid hydrolysis of)
RN 109923-29-7 HCAPLUS
CN α-D-Glucopyranose, 4-deoxy-4-fluoro-, 1-(dihydrogen phosphate), compd. with cyclohexanamine (1:2) (9CI) (CA INDEX NAME)

CM 1

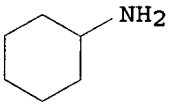
CRN 109923-28-6
CMF C6 H12 F O8 P

Absolute stereochemistry.



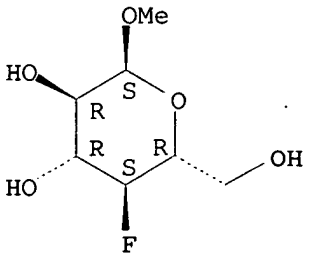
CM 2

CRN 108-91-8
CMF C6 H13 N



IT 56926-53-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 56926-53-5 HCAPLUS
CN α-D-Glucopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.

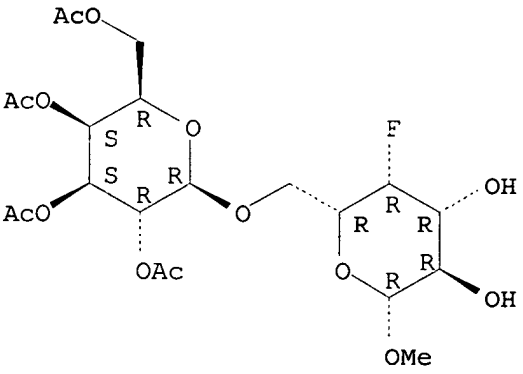


L24 ANSWER 55 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1985:79244 HCAPLUS
DOCUMENT NUMBER: 102:79244
ORIGINAL REFERENCE NO.: 102:12441a,12444a
TITLE: Synthesis of specifically fluorinated methyl β-glycosides of (1 → 6)-β-D-galactooligosaccharides. II. Methyl 4-deoxy-4-fluoro-6-O-(β-D-galactopyranosyl)-β-D-galactopyranoside
AUTHOR(S): Kovac, Pavol; Glaudemans, Cornelis P. J.
CORPORATE SOURCE: NIADDK, Bethesda, MD, 20205, USA
SOURCE: Journal of Carbohydrate Chemistry (1984), 3(2), 349-58
CODEN: JCACDM; ISSN: 0732-8303
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Condensation of Me 2,3-di-O-benzyl-4-deoxy-4-fluoro-β-D-galactopyranoside with 2,3,4,6-tetra-O-acetyl-α-D-galactopyranosyl bromide in the presence of Hg(CN)2 in benzene afforded, in excellent yield, the β-linked product, which was deblocked to give the title disaccharide.

IT 92397-30-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deacetylation of)
RN 92397-30-3 HCAPLUS
CN β-D-Galactopyranoside, methyl 4-deoxy-4-fluoro-6-O-(2,3,4,6-tetra-O-acetyl-β-D-galactopyranosyl)- (CA INDEX NAME)

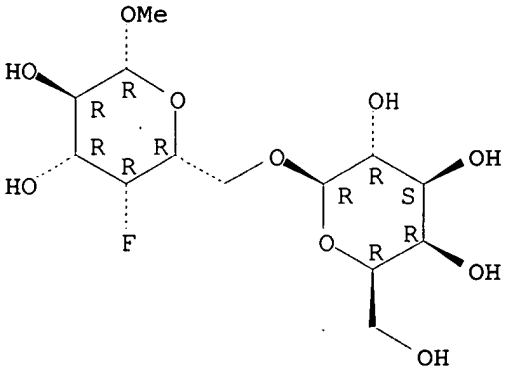
Absolute stereochemistry.



IT 92397-31-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 92397-31-4 HCAPLUS
CN β-D-Galactopyranoside, methyl 4-deoxy-4-fluoro-6-O-β-D-

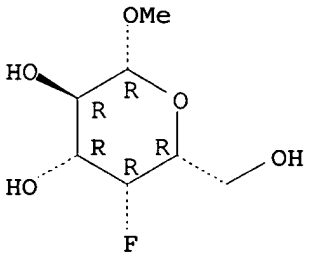
galactopyranosyl- (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 56 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1985:22521 HCAPLUS
DOCUMENT NUMBER: 102:22521
ORIGINAL REFERENCE NO.: 102:3709a,3712a
TITLE: Mapping of subsites in combining area of monoclonal anti-galactan immunoglobulin A, J539
AUTHOR(S): Glaudemans, Cornelis P. J.; Kovac, Pavol; Rasmussen, Kjeld
CORPORATE SOURCE: Natl. Inst. Arthritis, Diabetes, Dig. Kidney Dis., Bethesda, MD, 20205, USA
SOURCE: Biochemistry (1984), 23(26), 6732-6
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Monoclonal IgA J539 binds β(1→6)-D-galactopyranans. Measurement of the affinity of its Fab' fragment for a series of galacto oligosaccharides, some of which carried deoxyfluoro groups, has made it possible to assign a binding mode of the polysaccharide that has the reducing end oriented from the heavy (H) chains towards the light (L) chain. In addition, the values obtained for the affinity consts. of the Ig with these oligosaccharides, as well as the maximal values obtained for the intrinsic ligand-induced fluorescence, permit a deduction about the relative affinity of the protein's 4 subsites for each galactose residue of the tetrasaccharide fragment it can bind. If these subsites are labeled C, A, B, and D, going from the H-chain towards the L-chain across the face of the Ig combining area, then the order of decreasing affinity is A > B > C > D.
IT 51385-54-7
RL: BIOL (Biological study)
(monoclonal IgA binding to)
RN 51385-54-7 HCAPLUS
CN β-D-Galactopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



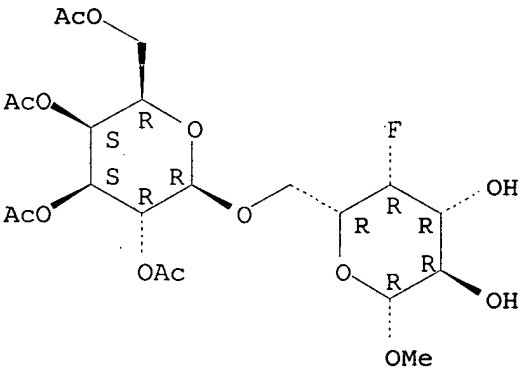
L24 ANSWER 57 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1984:611596 HCAPLUS
DOCUMENT NUMBER: 101:211596
ORIGINAL REFERENCE NO.: 101:32079a,32082a
TITLE: Carbon-13 and proton chemical shift assignments and proton-fluorine-19 spin-spin coupling constants in oligosaccharides and fluorinated oligosaccharides by two-dimensional carbon-13-proton chemical shift correlation spectroscopy with proton homonuclear decoupling
AUTHOR(S): Wong, Tuck C.; Rutar, Venceslav; Wang, Jin Shan; Feather, Milton; Kovac, Pavol
CORPORATE SOURCE: Dep. Chem., Univ. Missouri, Columbia, MO, 65211, USA
SOURCE: Journal of Organic Chemistry (1984), 49(23), 4358-63
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A version of the two-dimensional 13C-1H chemical shift correlation NMR spectroscopy which includes selective spin flip pulses has been used to resolve and assign 1H and 13C chemical shifts and to determine 1H-19F spin-spin couplings of a series of oligosaccharides and fluorinated oligosaccharides. The selective spin flip results in almost complete homonuclear decoupling in the 1H dimension, leading to substantially better resolution and signal to noise ratio.

IT 92397-30-3 92397-31-4
RL: PROC (Process)
(2-dimensional NMR of)

RN 92397-30-3 HCAPLUS
CN β-D-Galactopyranoside, methyl 4-deoxy-4-fluoro-6-O-(2,3,4,6-tetra-O-acetyl-β-D-galactopyranosyl)- (CA INDEX NAME)

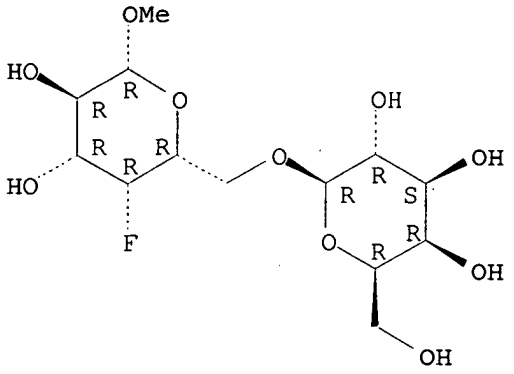
Absolute stereochemistry.



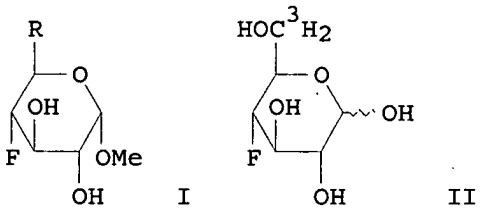
RN 92397-31-4 HCAPLUS
CN β-D-Galactopyranoside, methyl 4-deoxy-4-fluoro-6-O-β-D-

galactopyranosyl- (CA INDEX NAME)

Absolute stereochemistry.

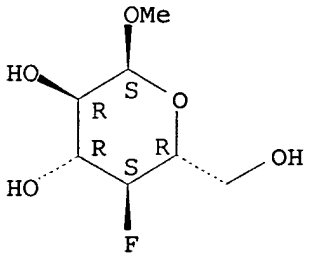


L24 ANSWER 58 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1984:611579 HCAPLUS
DOCUMENT NUMBER: 101:211579
ORIGINAL REFERENCE NO.: 101:32075a,32078a
TITLE: Synthesis of 4-deoxy-4-fluoro-D-[6-3H]glucose
AUTHOR(S): Samuel, John; Taylor, Norman Fletcher
CORPORATE SOURCE: Dep. Chem., Univ. Windsor, Windsor, ON, N9B 3P4, Can.
SOURCE: Carbohydrate Research (1984), 133(1), 168-72
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



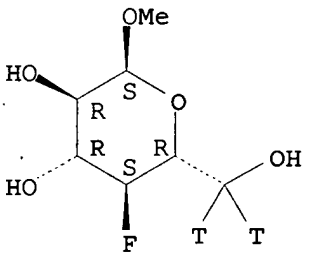
AB Oxidation of fluoroglucoside I (R = CH2OH) with O and Pt black, followed by treatment with CH2N2 gave uronate I (R = CO2Me), which on NaBT4 reduction gave labeled compound I (R = C3H2OH), which on acid hydrolysis gave the title compound (II). The total radiochem. yield from I (R = CO2Me) to II was 12.5%. Reoxidn. of I (R = C3H2OH) to I (R = CO2H) indicated that 96.3% of the T label was located at C-6 in II.
IT 56926-53-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of)
RN 56926-53-5 HCAPLUS
CN α-D-Glucopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



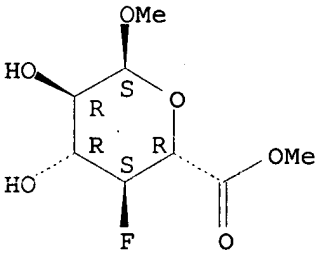
IT 93173-30-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acid hydrolysis of)
RN 93173-30-9 HCAPLUS
CN α-D-Glucopyranoside-6,6-C-t2, methyl 4-deoxy-4-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



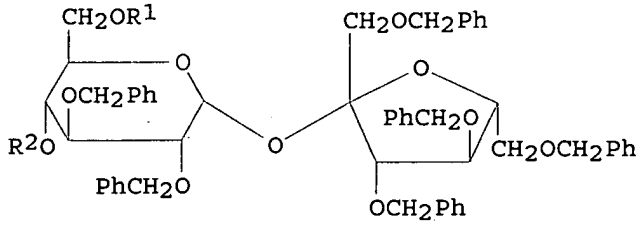
IT 93173-29-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of, with sodium borotritide)
RN 93173-29-6 HCAPLUS
CN α-D-Glucopyranosiduronic acid, methyl 4-deoxy-4-fluoro-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.

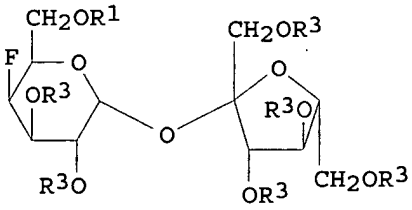


L24 ANSWER 59 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1984:592341 HCAPLUS
DOCUMENT NUMBER: 101:192341
ORIGINAL REFERENCE NO.: 101:29163a,29166a
TITLE: Sucrochemistry, part 35. The synthesis of some 4-deoxy-4-fluoro and 4,6-dideoxy-4,6-difluoro derivatives of sucrose
AUTHOR(S): Hough, Leslie; Kabir, Abul K. M. S.; Richardson, Anthony C.

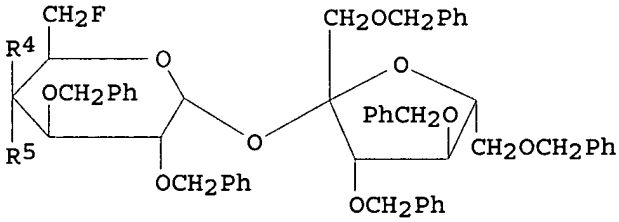
CORPORATE SOURCE: Dep. Chem., Queen Elizabeth Coll., London, W8 7AH, UK
SOURCE: Carbohydrate Research (1984), 131(2), 335-40
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II



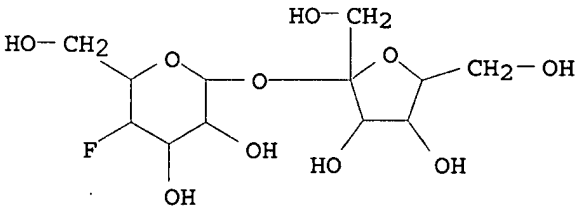
III

AB Sucrose derivative I (R1 = R2 = H) on tritylation followed by mesylation gave 61% I (R1 = trityl, R2 = mesyl), which on fluorination with Bu4NF in boiling MeCN for 3 days gave 65% fluoride II (R1 = trityl, R3 = PhCH2), which on deprotection by catalytic transfer hydrogenation gave fluorodeoxygalactosucrose II (R1 = R3 = H). Addnl. prepared were difluoro derivs. III (R4 = F, R5 = H; R4 = H, R5 = F) from I (R1 = R2 = H).

IT 92596-06-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acetylation of)

RN 92596-06-0 HCAPLUS

CN α-D-Galactopyranoside, β-D-fructofuranosyl 4-deoxy-4-fluoro- (9CI) (CA INDEX NAME)



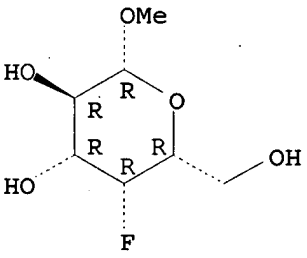
L24 ANSWER 60 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1984:139503 HCAPLUS
DOCUMENT NUMBER: 100:139503
ORIGINAL REFERENCE NO.: 100:21315a
TITLE: Carbon-13 NMR spectra of methyl deoxyfluoro-β-D-galactopyranosides and their per-O-acetyl derivatives
AUTHOR(S): Kovac, Pavol; Glaudemans, Cornelis P. J.
CORPORATE SOURCE: Natl. Inst. Arthritis, Diabetes, Dig. Kidney Dis., Bethesda, MD, 20205, USA
SOURCE: Journal of Carbohydrate Chemistry (1983), 2(3), 313-27
CODEN: JCACDM; ISSN: 0732-8303
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Me 6-deoxy-6-fluoro-β-D-galactopyranoside was obtained by treatment of Me β-D-galactopyranoside with diethylaminosulfur trifluoride. Improvements over the existing syntheses of Me 2,3-di-O-benzyl-4-deoxy-4-fluoro-β-D-galactopyranoside from the corresponding 6-O-substituted 4-O-arylsulfonyl-D-gluco derivs. are described. 13C NMR spectra of a series of Me deoxyfluoro-β-D-galactopyranosides and their per-O-acetyl derivs. were measured. The data obtained can be used as an aid for the interpretation of 13C NMR spectra of deoxyfluoro-β-D-galactopyranose-containing oligosaccharides and related substances.

IT 51385-54-7
RL: PRP (Properties)
(carbon-13 NMR of)
RN 51385-54-7 HCAPLUS
CN β-D-Galactopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.

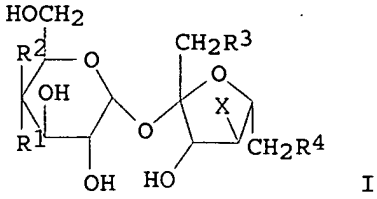


L24 ANSWER 61 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1984:33495 HCAPLUS
DOCUMENT NUMBER: 100:33495
ORIGINAL REFERENCE NO.: 100:5191a,5194a
TITLE: 4'-Halo-substituted sucrose derivatives
INVENTOR(S): Lee, Cheang K.
PATENT ASSIGNEE(S): Tate and Lyle PLC, UK
SOURCE: U.S., 15 pp. Cont.-in-part of U.S. Ser. No. 315,479, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 4405654	A	19830920	US 1982-371995		19820426 <--
ZA 8107425	A	19821027	ZA 1981-7425		19811027 <--
PRIORITY APPLN. INFO.:			GB 1980-34666	A	19801028
			GB 1981-25621	A	19810821

US 1981-315479 A2 19811027

GI

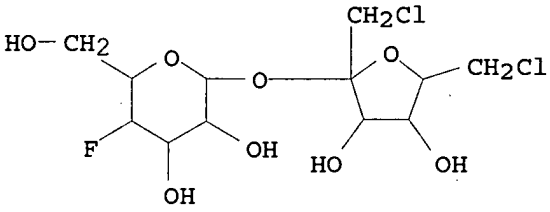


I

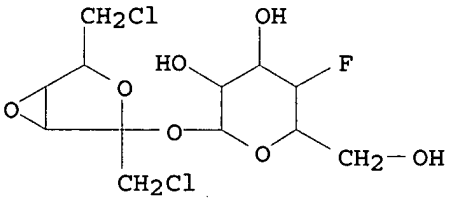
AB Compds. of general formula I, where R1 and R2 are H, OH, or halogen, R3 and R4 are OH or halogen, with at least 1 of R1, R2, and R3 being a halogen, may be used as sweetening agents for food. Thus, 4,1',6'-trichloro-4,1',6'-trideoxygalactosucrose (II) [56038-13-2] was reacted with tert-butyldiphenylsilyl chloride [58479-61-1] to form II 6-tert-butyldiphenylsilyl ether [82919-99-1]. The latter was reacted with Ph3P to form the 3',4'-lyxoepoxide which was then acetylated to form II 3',4'-lyxoepoxide triacetate [82920-02-3]. The latter was brominated and deacetylated to form 4'-bromo-4,1',6'-trichloro-4,4',1',6'-tetradeoxygalactosucrose [86172-31-8]. This compound was used as a soft drink sweetening agent.

IT 86172-53-4P 86172-54-5P 86172-55-6P
RL: PREP (Preparation)
(preparation of, in sweetening agent manufacture)

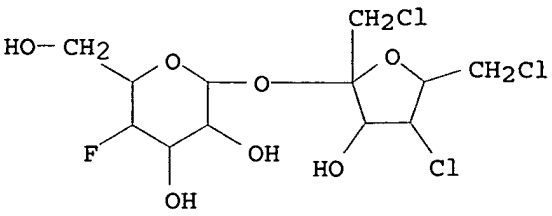
RN 86172-53-4 HCAPLUS
CN α-D-Galactopyranoside, 1,6-dichloro-1,6-dideoxy-β-D-fructofuranosyl 4-deoxy-4-fluoro- (9CI) (CA INDEX NAME)



RN 86172-54-5 HCAPLUS
CN α-D-Galactopyranoside, 3,4-anhydro-1,6-dichloro-1,6-dideoxy-β-D-tagatofuranosyl 4-deoxy-4-fluoro- (9CI) (CA INDEX NAME)



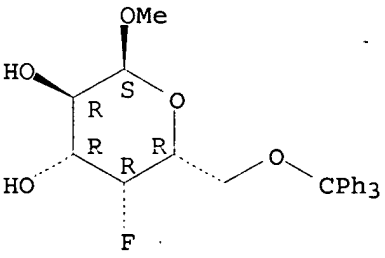
RN 86172-55-6 HCAPLUS
CN α-D-Galactopyranoside, 4-chloro-2,5-bis(chloromethyl)tetrahydro-3-hydroxy-2-furanyl 4-deoxy-4-fluoro-, [2R-(2α,3α,4β,5.alpha.)]- (9CI) (CA INDEX NAME)



RL: PREP (Preparation)
(sweetening agent, prepn. of

L24 ANSWER 62 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1984:22918 HCAPLUS
DOCUMENT NUMBER: 100:22918
ORIGINAL REFERENCE NO.: 100:3617a,3620a
TITLE: Stereo- and regio-selectivity of diethylaminosulfur trifluoride as a fluorinating reagent for methyl glycosides
AUTHOR(S): Somawardhana, Chandrasiri W.; Brunngraber, Eric G.
CORPORATE SOURCE: Dep. Biochem., Univ. Missouri Columbia, St. Louis, MO, 63139, USA
SOURCE: Carbohydrate Research (1983), 121, 51-60
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Me glycopyranosides reacted with diethylaminosulfur trifluoride (I) in the absence of solvent to yield Me dideoxydifluoro and deoxyfluoro glycopyranosides. Me α-D-glycopyranosides produced 6-deoxy-6-fluoro- and 4,6-dideoxy-4,6-difluoro derivs. with Walden inversion at C-4. Me β-D-glucopyranoside also produced a 3,6-dideoxy-3,6-difluoro derivative, with Walden inversion at C-3. Me 6-O-trityl-α-D-glucopyranoside, reacted with I to yield the corresponding 4-deoxy-4-fluorogalactopyranoside derivative
IT 87586-00-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 87586-00-3 HCAPLUS
CN α-D-Galactopyranoside, methyl 4-deoxy-4-fluoro-6-O-(triphenylmethyl)- (CA INDEX NAME)

Absolute stereochemistry.



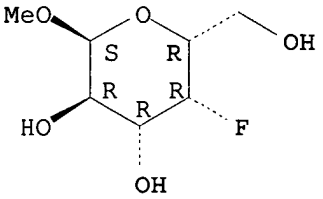
L24 ANSWER 63 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1983:612837 HCAPLUS
DOCUMENT NUMBER: 99:212837
ORIGINAL REFERENCE NO.: 99:32767a,32770a
TITLE: Fluorinated carbohydrates. 2. Selective fluorination of gluco- and mannopyranosides. Use of 2-D NMR for structural assignments
AUTHOR(S): Card, Peter J.; Reddy, Gade S.

CORPORATE SOURCE: Cent. Res. Dev. Dep., E. I. du Pont de Nemours and Co., Wilmington, DE, 19898, USA
SOURCE: Journal of Organic Chemistry (1983), 48(24), 4734-43
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Me and Ph α-glucosides, or suitably protected derivs., may be selectively fluorinated with Et2NSF3 at the 4- or 6-position to afford the corresponding fluorinated galacto- or glucopyranoside. Unlike the α-glucosides, β-glucosides were fluorinated at C-3 to give the 3-deoxy-3-fluoro-β-allo derivs. High yields of primary fluorinated (C-6) products were obtained from both α- and β-glucosides by use of appropriate reaction times. Use of 6-O-trityl derivs. of Me α- and β-glucosides gave Me 4-deoxy-4-fluoro-α-galactopyranoside and Me 3-deoxy-3-fluoro-β-allopyranoside, resp. Fluorinated p-nitrophenyl α- and β-gluco- and -galactopyranosides were also prepared using Et2NSF3. 6-O-Pivaloate esters of Me α-gluco- and α- and β-galactopyranosides were prepared as acid and Et2NSF3-stable 6-O protecting groups. An intramol. fluoride-ion delivery mechanism for the SN2 displacement reaction at C-4 in Me α-D-mannopyranoside was shown. Me 4-amino-4,6-dideoxy-6-fluoro-α-D-glucopyranoside, Me 6-amino-3,6-dideoxy-3-fluoro-β-D-allopyranoside, and Me 6-amino-4,6-dideoxy-4-fluoro-α-D-talopyranoside were similarly prepared

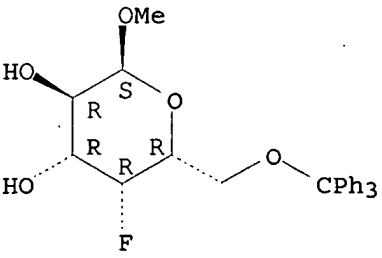
IT 32934-07-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acetylation of)
RN 32934-07-9 HCAPLUS
CN α-D-Galactopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



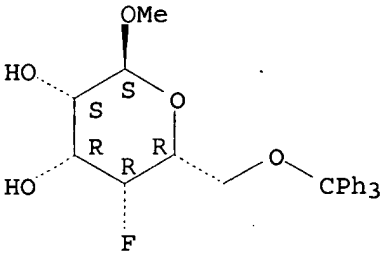
IT 87586-00-3P 87586-11-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and detritylation of)
RN 87586-00-3 HCAPLUS
CN α-D-Galactopyranoside, methyl 4-deoxy-4-fluoro-6-O-(triphenylmethyl)- (CA INDEX NAME)

Absolute stereochemistry.



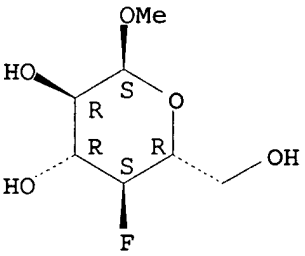
RN 87586-11-6 HCAPLUS
CN α-D-Talopyranoside, methyl 4-deoxy-4-fluoro-6-O-(triphenylmethyl)- (CA INDEX NAME)

Absolute stereochemistry.



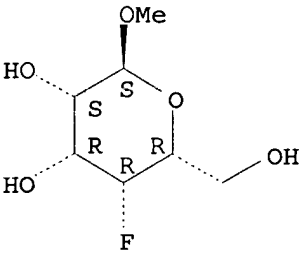
IT 56926-53-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and fluorination of, with (diethylamino)sulfur trifluoride)
RN 56926-53-5 HCAPLUS
CN α-D-Glucopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



IT 87586-12-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 87586-12-7 HCAPLUS
CN α-D-Talopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



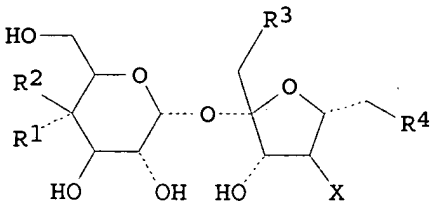
L24 ANSWER 64 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1983:454127 HCAPLUS
DOCUMENT NUMBER: 99:54127
ORIGINAL REFERENCE NO.: 99:8469a
TITLE: 4'-Halo-substituted sucrose derivatives
INVENTOR(S): Jackson, Graham; Jenner, Michael Ralph; Khan, Riaz

Ahmed; Lee, Cheang Kuan; Mufti, Khizar Sultan; Patel, Gita Dilip; Rathbone, Elner Brean

PATENT ASSIGNEE(S): Tate and Lyle PLC, UK
SOURCE: Eur. Pat. Appl., 54 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 73093	A1	19830302	EP 1982-302047	19820421 <--
EP 73093	B1	19841024		
R: AT, BE, CH, DE, FR, IT, LI, LU, NL, SE				
GB 2104063	A	19830302	GB 1982-11477	19820421 <--
GB 2104063	B	19851106		
AT 10003	T	19841115	AT 1982-302047	19820421 <--
NO 8201348	A	19830222	NO 1982-1348	19820426 <--
NO 152875	B	19850826		
NO 152875	C	19851204		
IL 65621	A	19850830	IL 1982-65621	19820426 <--
SU 1301316	A3	19870330	SU 1982-3427200	19820426 <--
DK 8201887	A	19830222	DK 1982-1887	19820427 <--
DK 158472	B	19900521		
DK 158472	C	19901008		
AU 8283025	A	19830224	AU 1982-83025	19820427 <--
AU 557186	B2	19861211		
JP 58035196	A	19830301	JP 1982-71130	19820427 <--
JP 62054436	B	19871114		
ZA 8202854	A	19830330	ZA 1982-2854	19820427 <--
ES 511753	A1	19830601	ES 1982-511753	19820427 <--
CA 1189070	A1	19850618	CA 1982-401740	19820427 <--
FI 8201486	A	19830222	FI 1982-1486	19820428 <--
FI 71159	B	19860814		
FI 71159	C	19861124		

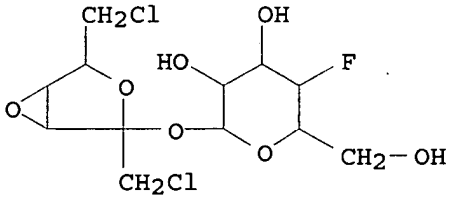
PRIORITY APPLN. INFO.: GB 1981-25622 A 19810821
EP 1982-302047 A 19820421
OTHER SOURCE(S): MARPAT 99:54127
GI



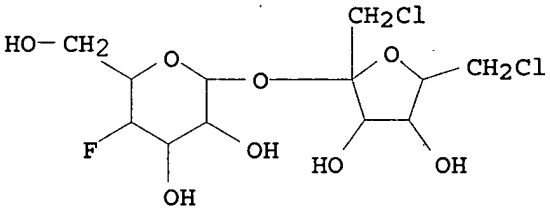
I

AB Sucrose derivs. I [X = halo; R1 and R2 resp. = OH and H, halo and H, or H and halo, R3 and R4 (same or different) = halo or OH; at least one of R1, R2, and R3 = halo] were prepared I have sweetness <7500 times that of sucrose and are devoid of unpleasant bitter, metallic and lingering aftertaste. Thus, 4,1',6'-trichloro-4,1',6'-trideoxygalactosucrose (II) was treated with di-Et azodicarboxylate and Ph3P in PhMe and then acetylated to give II-3',4'-lyxo-epoxide triacetate, which was treated with LiCl in DMF at 90° for 5 h and then acetylated to give 4,1',4',6'-tetrachloro-4,1',4',6'-tretradeoxygalactosucrose (III) tetraacetate, which was deacetylated to III.
IT 86172-54-5P

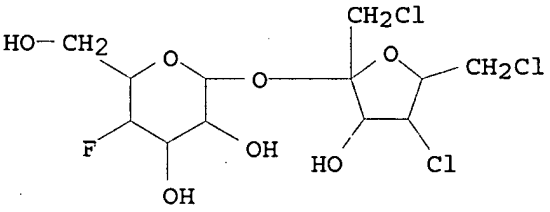
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and chlorination of)
RN 86172-54-5 HCAPLUS
CN α-D-Galactopyranoside, 3,4-anhydro-1,6-dichloro-1,6-dideoxy-β-D-tagatofuranosyl 4-deoxy-4-fluoro- (9CI) (CA INDEX NAME)



IT 86172-53-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion of, to epoxide derivative)
RN 86172-53-4 HCAPLUS
CN α-D-Galactopyranoside, 1,6-dichloro-1,6-dideoxy-β-D-fructofuranosyl 4-deoxy-4-fluoro- (9CI) (CA INDEX NAME)



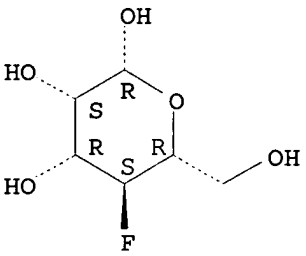
IT 86172-55-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 86172-55-6 HCAPLUS
CN α-D-Galactopyranoside, 4-chloro-2,5-bis(chloromethyl)tetrahydro-3-hydroxy-2-furanyl 4-deoxy-4-fluoro-, [2R-(2α,3α,4β,5.alph a.)]- (9CI) (CA INDEX NAME)



L24 ANSWER 65 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1983:438721 HCAPLUS
DOCUMENT NUMBER: 99:38721
ORIGINAL REFERENCE NO.: 99:6101a,6104a
TITLE: Synthesis of 3-deoxy-3-fluoro-D-mannose and 4-deoxy-4-fluoro-D-mannose
AUTHOR(S): Rasmussen, James R.; Tafuri, Sherrie R.; Smale, Stephen T.
CORPORATE SOURCE: Dep. Chem., Cornell Univ., Ithaca, NY, 14853, USA
SOURCE: Carbohydrate Research (1983), 116(1), 21-9

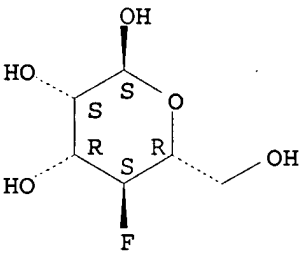
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Addition of KCN to 2-deoxy-2-fluoro-D-arabinose at pH 7.8 followed by catalytic hydrogenation over Pd/BaSO4 (5%) produced 3-deoxy-3-fluoro-D-glucose and 3-deoxy-3-fluoro-D-mannose in 25 and 40% isolated yields, resp. The epimeric sugars were purified by passage through a column of Dowex-50W + 8 (Ca2+). In a similar manner, 3-deoxy-3-fluoro-D-arabinose was converted into 4-deoxy-4-fluoro-D-glucose and 4-deoxy-4-fluoro-D-mannose in 27 and 45% isolated yields, resp. Deoxyfluorohexoses enriched with carbon-13 and carbon-14 at C-1 have been prepared by this procedure.
IT 86258-32-4P 86258-33-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 86258-32-4 HCAPLUS
CN β-D-Mannopyranose, 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



RN 86258-33-5 HCAPLUS
CN α-D-Mannopyranose, 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



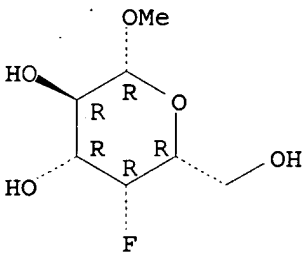
L24 ANSWER 66 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1981:587597 HCAPLUS
DOCUMENT NUMBER: 95:187597
ORIGINAL REFERENCE NO.: 95:31321a,31324a
TITLE: Preparation of two methyl deoxyfluoro-β-D-galactopyranosides, and their interaction with galactan-specific immunoglobulin A J539 (Fab')
AUTHOR(S): Ittah, Yitzhak; Glaudemans, Cornelis P. J.
CORPORATE SOURCE: Natl. Inst. Arthritis, Metab. Dig. Dis., Bethesda, MD, 20205, USA
SOURCE: Carbohydrate Research (1981), 95(2), 189-94
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Me 2-deoxy-2-fluoro-β-D-galactopyranoside (I) and Me

4-deoxy-4-fluoro-β-D-galactopyranoside (II) were prepared, and the possibility of their binding to (1→6)-β-D-galactopyranan-specific IgA J539 (Fab') was investigated. I does not show binding, whereas II does. The 2-OH group of Me β-D-galactopyranoside may take part in H bonding to the protein.

IT 51385-54-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and interaction of, with IgA J539)

RN 51385-54-7 HCAPLUS
CN β-D-Galactopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



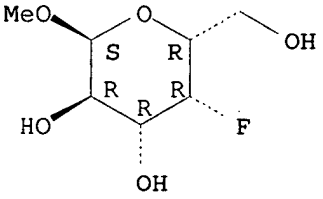
L24 ANSWER 67 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1980:633690 HCAPLUS
DOCUMENT NUMBER: 93:233690
ORIGINAL REFERENCE NO.: 93:37323a,37326a
TITLE: Specificity of α- and β-D-galactosidase towards analogs of D-galactopyranosides modified at C-4 or C-5
AUTHOR(S): Shin, Jeong E. Nam; Maradufu, Asafu; Marion, Jean; Perlin, Arthur S.
CORPORATE SOURCE: Dep. Chem., McGill Univ., Montreal, QC, H3C 3G1, Can.
SOURCE: Carbohydrate Research (1980), 84(2), 328-35
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 4-Deoxy analogs of Me α- and β-D-galactopyranoside were prepared None of the 4-deoxy or the 5-thio analogs were substrates for either β-D-galactosidase (I) from Escherichia coli or α-D-galactosidase from Aspergillus fumigatus. The 4-deoxy-4-fluoro-analog was a competitive inhibitor of I and the 4-amino-4-deoxy analog was a noncompetitive inhibitor. Thus, the 4-OH group of D-galactose seems to uniquely satisfy both the spatial and H-bonding requirements of the activated enzymes.

IT 32934-07-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and α-galactosidase inhibition by)

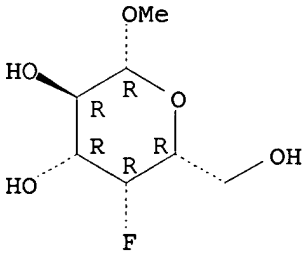
RN 32934-07-9 HCAPLUS
CN α-D-Galactopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



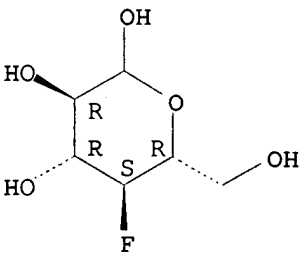
IT 51385-54-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and β-galactosidase inhibition by)
RN 51385-54-7 HCAPLUS
CN β-D-Galactopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



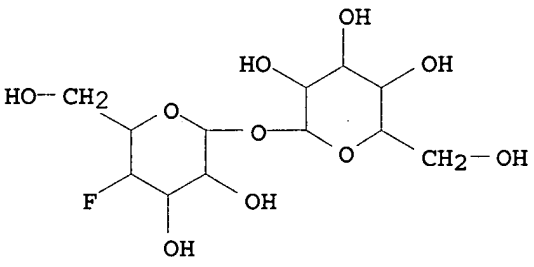
L24 ANSWER 68 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1979:606294 HCAPLUS
DOCUMENT NUMBER: 91:206294
ORIGINAL REFERENCE NO.: 91:33187a,33190a
TITLE: The substrate specificity of yeast hexokinase: reaction with D-arabinose oxime
AUTHOR(S): Finch, Paul; Merchant, Zohar M.
CORPORATE SOURCE: Bourne Lab., R. Holloway Coll., Egham/Surrey, TW20 OEX, UK
SOURCE: Carbohydrate Research (1979), 76, 225-32
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English
AB By chromatog., electrophoresis, NMR spectroscopy, and spectrophotometric assay, D-arabinose oxime (I) was shown to act as a weak substrate for yeast hexokinase (II). II-catalyzed phosphorylation of I, which was present as a mixture of 80% E- and 20% Z-acyclic forms in solution at equilibrium, was proposed to proceed via the transient formation of a furanoid species. Weak substrate activity was also observed with 4-deoxy-D-xylo-hexose, but not with 5-deoxy-D-xylo-hexose. The relation of these and previous results concerning the carbohydrate substrate specificity of yeast II in solution to x-ray crystallog. studies is discussed.
IT 30694-44-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with hexokinase, kinetics of)
RN 30694-44-1 HCAPLUS
CN D-Glucopyranose, 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 69 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1979:457338 HCAPLUS
DOCUMENT NUMBER: 91:57338
ORIGINAL REFERENCE NO.: 91:9310h,9311a
TITLE: Chemical modification of trehalose: Part XXI. The syntheses of 4,6-dideoxy-4,6-difluoro- and 4-deoxy-4-fluoro-α,α-trehalose
AUTHOR(S): Hadfield, Anthony F.; Hough, Leslie; Richardson, Anthony C.
CORPORATE SOURCE: Queen Elizabeth Coll., Univ. London, London, W8 7AH, UK
SOURCE: Carbohydrate Research (1979), 71, 95-102
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Prolonged treatment of 2,3-di-O-mesyl-α-D-glucopyranosyl 2,3-di-O-benzylidene-α-D-glucopyranoside with Bu4N+F- in MeCN gave 71% 4,6-difluoride, from which 4,6-dideoxy-4,6-difluoro-α-D-galactopyranosyl α-D-glucopyranoside was prepared In a similar reaction with 2,3-di-O-benzyl-4,6-di-O-mesyl-α-D-galactopyranosyl 2,3-di-O-benzyl-4,6-O-benzylidene-α-D-glucopyranoside, two products were formed, as indicated by the 19F-NMR spectrum of the reaction mixture, and tentatively identified as the required 4,6-difluoride and the 6-fluoro-4-ene. Fluoride displacement of the mesyloxy group of 2,3-di-O-benzyl-4-O-mesyl-6-O-trityl-α-D-glucopyranosyl 2,3-di-O-benzyl-4,6-O-benzylidene-α-D-glucopyranoside readily gave the 4-fluoride which, on deprotection, gave 4-deoxy-4-fluoro-α-D-galactopyranosyl α-D-glucopyranoside.
IT 70836-41-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acetylation of)
RN 70836-41-8 HCAPLUS
CN α-D-Galactopyranoside, α-D-glucopyranosyl 4-deoxy-4-fluoro- (9CI) (CA INDEX NAME)



L24 ANSWER 70 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1978:595232 HCAPLUS
DOCUMENT NUMBER: 89:195232
ORIGINAL REFERENCE NO.: 89:30335a,30338a
TITLE: Binding studies on β-D-galactopyranosyl antibodies. Intramolecular hydrogen bonding effects
AUTHOR(S): Lemieux, R. U.; Boullanger, P. H.; Bundle, D. R.; Baker, D. A.; Nagpurkar, A.; Venot, A.
CORPORATE SOURCE: Dep. Chem., Univ. Alberta, Edmonton, AB, Can.
SOURCE: Nouveau Journal de Chimie (1978), 2(4), 321-9
CODEN: NJCHD4; ISSN: 0398-9836
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Antibodies raised in rabbit against (β-D-galactopyranosyl-O

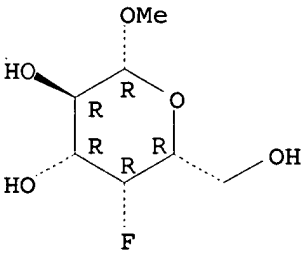
(CH2)8CONH)24-bovine serum albumin were purified by affinity chromatog. and quant. inhibitions of the precipitation of the antibodies by the immunizing antigen by a large number of structures related to the haptenic structure were determined The results appear to require that the β-D-galactopyranosyl group binds in an extensively intramol. hydrogen bonded form and that binding of the aliphatic aglycon beyond the 2nd methylene group is basically the result of random, non-specific hydrophobic bonding. Intramol. hydrogen bonding may provide an important mechanism for the binding of carbohydrate structures to hydrophobic surfaces.

IT 51385-54-7
RL: BIOL (Biological study)
(hapten, galactopyranosyl antibody binding of, intermol. hydrogen bonding in)

RN 51385-54-7 HCAPLUS

CN β-D-Galactopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 71 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1977:106915 HCAPLUS

DOCUMENT NUMBER: 86:106915

ORIGINAL REFERENCE NO.: 86:16880h,16881a

TITLE: The carbon-13 nuclear magnetic resonance spectra of the deoxyfluoro-D-glucoses, 2-deoxy-2-fluoro-D-mannose, and 4-deoxy-4-fluoro-D-galactose. Orientational and substituent effects upon nJFC

AUTHOR(S): Wray, Victor

CORPORATE SOURCE: Ges. Molekularbiol. Forsch. mbH, Braunschweig, Fed. Rep. Ger.

SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1976), (13), 1598-605
CODEN: JCPKBH; ISSN: 0300-9580

DOCUMENT TYPE: Journal

LANGUAGE: English

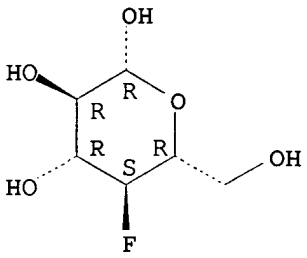
AB The 13C NMR spectra of the anomeric pairs of the deoxyfluoro-D-glucopyranoses, 2-deoxy-2-fluoro-D-mannopyranose, and 4-deoxy-4-fluoro-D-galactose were studied to investigate the effects of substituents upon JFC values. The variation in 1JFC with the electronegativity of α-substituents was rationalized. 2JFC although less dependent upon the electronegativity of substituents attached to the coupled fragment, depends upon the orientation of substituents bonded to the coupled C. 3JFC and 4JFC depend on the orientation of the coupled nuclei and 3JFC depends on the orientation of substituents on the coupled fragment. The angular dependence of 3JFC and 4JFC and their dependence on the angular disposition of electroneg. substituents is reproduced by INDO MO calcns.

IT 27108-04-9 32934-09-1 32934-10-4
62182-11-0
RL: PRP (Properties)
(carbon-13 NMR of)

RN 27108-04-9 HCAPLUS

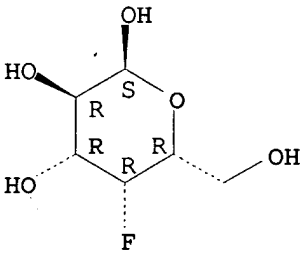
CN β-D-Glucopyranose, 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



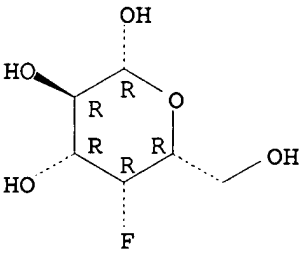
RN 32934-09-1 HCAPLUS
CN α-D-Galactopyranose, 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



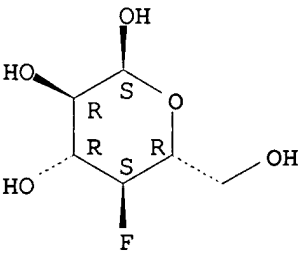
RN 32934-10-4 HCAPLUS
CN β-D-Galactopyranose, 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



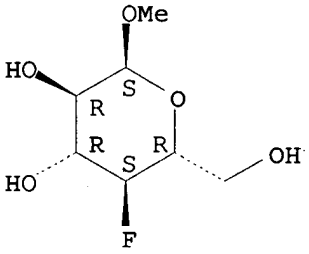
RN 62182-11-0 HCAPLUS
CN α-D-Glucopyranose, 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 72 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1975:571188 HCAPLUS
DOCUMENT NUMBER: 83:171188
ORIGINAL REFERENCE NO.: 83:26799a,26802a
TITLE: Methyl 4-deoxy-4-fluoro-α-D-glucopyranoside, C7H13FO5
AUTHOR(S): Choong, W.; Stephenson, N. C.; Stevens, J. D.
CORPORATE SOURCE: Sch. Chem., Univ. New South Wales, Kensington, Australia
SOURCE: Crystal Structure Communications (1975), 4(3), 491-6
CODEN: CSCMCS; ISSN: 0302-1742
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The effect on the mol. structure by replacing the OH group at the C(4) position of Me α-D-glucopyranoside by a F was studied by x-ray diffraction. The crystals of the title compound are orthorhombic, space group P212121, with a 8.415, b 13.827, and c 7.347 Å; d.(observed) = 1.52 and d.(calculated) = 1.52 for Z = 4. The structure was solved by direct methods with the program MULTAN 74 and by Fourier synthesis. The refinement was by full-matrix least-squares procedures to an R of 0.028. The mol. has 4C1 conformation with all bond lengths identical to those of methyl α-D-glucopyranoside except the C(6)-O(6) bond is shorter. Where O(6) is gauche to O(5) and trans to C(4) in methyl α-D-glucopyranoside, O(6) is gauche to both in this mol. structure. The H-bonding scheme is different.
IT 56926-53-5
RL: PRP (Properties)
(crystal structure of)
RN 56926-53-5 HCAPLUS
CN α-D-Glucopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.

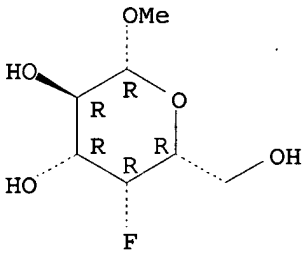


L24 ANSWER 73 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1974:96295 HCAPLUS
DOCUMENT NUMBER: 80:96295
ORIGINAL REFERENCE NO.: 80:15499a,15502a
TITLE: Synthesis of analogs of methyl β-D-galactopyranoside modified at C-4
AUTHOR(S): Maradufu, Asafu; Perlin, Arthur S.
CORPORATE SOURCE: Dep. Chem., McGill Univ., Montreal, QC, Can.
SOURCE: Carbohydrate Research (1974), 32(2), 261-77
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 80:96295
AB Me β-D-galactopyranosides (the 4-amino-4-deoxy, 4-azido-4-deoxy, 4-bromo-4-deoxy, 4-chloro-4-deoxy, 4-deoxy-4-fluoro, 4-deoxy-4-iodo, and 4-thio derivs.) potential substrates for D-galactose oxidase were prepared

by nucleophilic displacement of the 4-(p-bromophenylsulfonyl)oxy group of the appropriate D-glucose derivs. The (trifluoromethylsulfonyl)oxy group was also utilized as a novel leaving-group. Formation of the bromo and iodo derivs. was accompanied by appreciable halogen exchange and a resulting overall retention of configuration, and formation of the thio compound was attended by competing reactions. Optical rotatory characteristics of the halogeno compounds, their triacetates, and tribenzoates are described, and the anomalous behavior of the last group is noted.

IT 51385-54-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 51385-54-7 HCAPLUS
CN β-D-Galactopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.

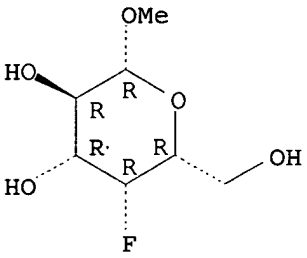


L24 ANSWER 74 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1974:79597 HCAPLUS
DOCUMENT NUMBER: 80:79597
ORIGINAL REFERENCE NO.: 80:12795a,12798a
TITLE: Nonhydrogen-bonding role for the 4-hydroxyl group of D-galactose in its reaction with D-galactose oxidase
AUTHOR(S): Maradufu, Asafu; Perlin, Arthur S.
CORPORATE SOURCE: Dep. Chem., McGill Univ., Montreal, QC, Can.
SOURCE: Carbohydrate Research (1974), 32(1), 93-9
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Several 4-deoxy analogs of Me β-D-galactopyranoside are oxidized by D-galactose oxidase. The rates associated with their various, axially attached 4-substituents follow the sequence OH>NH2>F>>Cl>H; these differences are attributed mainly to variations in Km. Other 4-deoxy analogs, namely, the 4-azido-4-deoxy, 4-bromo-4-deoxy-, 4-deoxy-4-iodo, and 4-thio derivs. were inactive. These observations indicate that the axial 4-hydroxyl group of D-galactopyranose does not play a H-bonding role primarily, but constitutes a substituent of a size optimal for interaction with the enzyme.

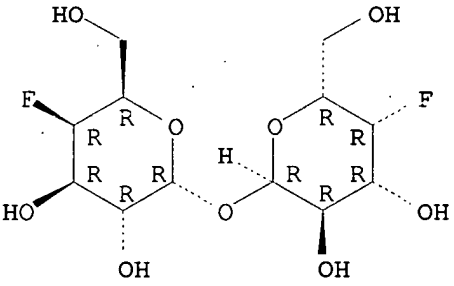
IT 51385-54-7
RL: BIOL (Biological study)
(reaction with galactose oxidase, kinetics of)
RN 51385-54-7 HCAPLUS
CN β-D-Galactopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 75 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1973:148162 HCAPLUS
DOCUMENT NUMBER: 78:148162
ORIGINAL REFERENCE NO.: 78:23825a,23828a
TITLE: Chemical modification of trehalose. XIII. Synthesis of 4,4'-difluoro and 4,4',6,6'-tetrafluoro analogs
AUTHOR(S): Hough, Leslie; Palmer, Anthony K.; Richardson, Anthony C.
CORPORATE SOURCE: Dep. Chem., Queen Elizabeth Coll., London, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1973), No. 8, 784-8
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB 2,3-Di-O-benzyl-4-O-(methylsulfonyl)-6-O-(triphenylmethyl -α-D-glucopyranoside (I) and 2,3-di-O-benzoyl-4,6-bis-O-(methylsulfonyl)-α-D-glucopyranoside (II) with Bu4NF gave, after removal of the protecting groups, the 4-deoxy-4fluoro-and 4,6-dideoxy-4,6-difluoro-galacto analogs (III, R = OH and F resp.) in 21% yield. The galacto analogs of I and II with Bu4NF gave the corresponding gluco fluorinated compds. in low yield, extensive elimination also occurring.
IT 41548-17-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 41548-17-8 HCAPLUS
CN α-D-Galactopyranoside, 4-deoxy-4-fluoro-α-D-galactopyranosyl 4-deoxy-4-fluoro- (9CI) (CA INDEX NAME)

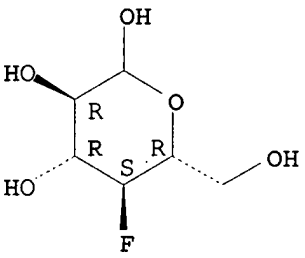
Absolute stereochemistry.



L24 ANSWER 76 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1971:488856 HCAPLUS
DOCUMENT NUMBER: 75:88856
ORIGINAL REFERENCE NO.: 75:14085a,14088a
TITLE: Stereospecific electronegative effects. I. Fluorine-19 nuclear magnetic resonance spectra of

deoxyfluoro-D-glucopyranoses
AUTHOR(S): Phillips, L.; Wray, V.
CORPORATE SOURCE: Org. Chem. Dep., Imp. Coll. Sci. Technol., London, UK
SOURCE: Journal of the Chemical Society [Section] B: Physical Organic (1971), (8), 1618-24
CODEN: JCSPAC; ISSN: 0045-6470
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 19F NMR spectra of the anomeric pairs of 1-deoxy-1-fluoro-, 2-deoxy-2-fluoro- (I), 3-deoxy-3-fluoro-, 4-deoxy-4-fluoro- (II), and 6-deoxy-6-fluoro-D-glueoses (III), and 2-deoxy-2-fluoro-D-mannose in D2O were determined The configurations and conformations of the mols. were determined from the geminal and vicinal 19F-1H spin-spin coupling consts., PMR parameters, and observed equilibrium anomer concns. The small vicinal 19F-1H coupling consts. of I and II were rationalized in terms of the electronegativity of the ring O, and the gauche 19F-1H coupling consts. were calculated The large (27 Hz) F coupling to H-5 in III indicates a favored rotational isomer in which F-6 is antiparallel to H-5. Vicinal 19F-1H coupling has a stereochem. dependence upon electroneg. substituents, and the 19F chemical shifts and chemical shift differences between pairs of anomers were explained by stereochem. dependence upon electroneg. substituents elsewhere in the mol.
IT 30694-44-1
RL: PRP (Properties)
(nuclear magnetic resonance of, configuration in relation to)
RN 30694-44-1 HCAPLUS
CN D-Glucopyranose, 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.

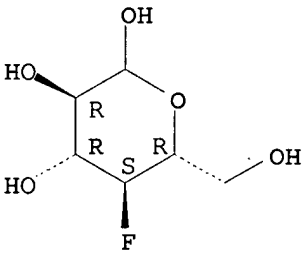


L24 ANSWER 77 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1971:464130 HCAPLUS
DOCUMENT NUMBER: 75:64130
ORIGINAL REFERENCE NO.: 75:10175a,10178a
TITLE: Specifically fluorinated carbohydrates. XIV. Fluorinated carbohydrates. XII. 4-Deoxy-4-fluoro-D-glucose. Improved synthesis and the glycosyl fluoride derivatives
AUTHOR(S): Barford, A. D.; Foster, A. B.; Westwood, J. H.; Hall, L. D.; Johnson, R. N.
CORPORATE SOURCE: Chester Beatty Res. Inst., R. Cancer Hosp., London, UK
SOURCE: Carbohydrate Research (1971), 19(1), 49-61
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 75:64130
AB 4-Deoxy-4-fluoro-D-glucose (I) was prepared Treatment of 1,6-anhydro-4-O-tosyl-β-D-glucopyranose or 1,6:3,4-dianhydro-β-D-galactopyranose (II) with potassium hydrogen fluoride in boiling 1,2-ethanediol affords 1,6-anhydro-4-deoxy-4-fluoro-β-D-glucopyranose (III). Acid hydrolysis effects the conversion of III to I. The

dianhydride II was obtained by photolysis of its 2-O-tosyl derivative NMR data were given for I and the 3-fluoro analog, and for 2,3,6-tri-O-acetyl-4-deoxy-4-fluoro-α-and -β-D-glucopyranosyl fluoride. Numerous long range (4J and 5J) F-H and F-F couplings were observed Treatment of the 2-p-toluenesulfonate of III with base gave 1,6.2:3-dianhydro-4-deoxy-4-fluoro-β-D-mannopyranose, which was converted into 1,6-anhydro-2,4-dideoxy-2,4-difluoro-β-D-glucopyranose by reaction with potassium hydrogen fluoride.

IT 30694-44-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 30694-44-1 HCAPLUS
CN D-Glucopyranose, 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.

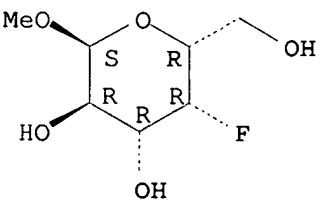


L24 ANSWER 78 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1971:436515 HCAPLUS
DOCUMENT NUMBER: 75:36515
ORIGINAL REFERENCE NO.: 75:5785a,5788a
TITLE: Fluorinated carbohydrates. IV. 4-Deoxy-4-fluoro-D-galactose
AUTHOR(S): Marcus, Donald M.; Westwood, J. H.
CORPORATE SOURCE: Inst. Cancer Res., R. Cancer Hosp., London, UK
SOURCE: Carbohydrate Research (1971), 17(2), 269-74
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English

AB When Me 2,3-di-O-benzyl-4-O-mesyl-6-O-trityl-α-D-glucopyranoside was treated with Bu4N+F- in boiling MeCN, a slow displacement of the equatorial mesyloxy group by fluoride occurred, with Walden inversion, yielding the resp. 4-deoxy-4-fluoro-D-galactose derivative On hydrogenolysis and acid hydrolysis the title compound was obtained.

IT 32934-07-9P 32934-09-1P 32934-10-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 32934-07-9 HCAPLUS
CN α-D-Galactopyranoside, methyl 4-deoxy-4-fluoro- (CA INDEX NAME)

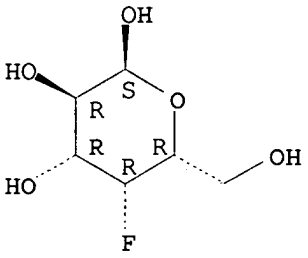
Absolute stereochemistry. Rotation (+).



RN 32934-09-1 HCAPLUS

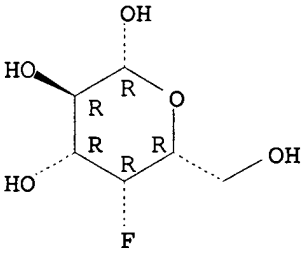
CN α-D-Galactopyranose, 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



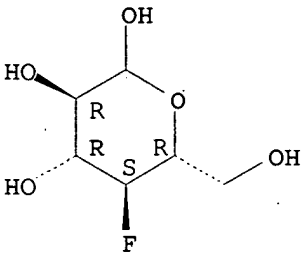
RN 32934-10-4 HCAPLUS
CN β-D-Galactopyranose, 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 79 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1971:23076 HCAPLUS
DOCUMENT NUMBER: 74:23076
ORIGINAL REFERENCE NO.: 74:3743a,3746a
TITLE: Fluorinated carbohydrates. II. Alternative syntheses of 4-deoxy-4-fluoro-D-glucose
AUTHOR(S): Foster, Allan B.; Hems, R.; Westwood, J. H.
CORPORATE SOURCE: Chester Beatty Res. Inst., R. Cancer Hosp., London, UK
SOURCE: Carbohydrate Research (1970), 15(1), 41-9
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 74:23076
GI For diagram(s), see printed CA Issue.
AB Treatment of Me 4-O-mesyl-2,3-di-O-methyl-6-O-trityl-α-D-galactopyranoside (I, R = CPh3) with Bu4N+F- in boiling MeCN and of Me 4-O-mesyl-2,3-di-O-methyl-α-D-galactopyranoside (I, R = H) with CsF in boiling HOCH2CH2OH gave II(R = CPh3) and II (R = H), resp., which are derivs. of 4-deoxy-4-fluoro-D-glucopyranose. These reactions were the 1st examples of the direct F- displacement of pyranose secondary sulfonates. Demethylation of Me 4-deoxy-4-fluoro-2,3-di-O-methyl-α-D-glucopyranoside (II, R = H) with BCl3 gave 4-deoxy-4-fluoro-D-glucose. NMR data for II(R = H) revealed a long-range (5J) coupling (3-4 Hz) between F-4 and H-1. The mass-spectral fragmentation pattern of II(R = Ac) was discussed.
IT 30694-44-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 30694-44-1 HCAPLUS
CN D-Glucopyranose, 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 80 OF 80 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1970:55785 HCAPLUS
DOCUMENT NUMBER: 72:55785
ORIGINAL REFERENCE NO.: 72:10236h,10237a
TITLE: 4-Deoxy-4-fluoro-D-glucose
AUTHOR(S): Barford, A. D.; Foster, A. B.; Westwood, J. H.
CORPORATE SOURCE: Roy. Cancer Hosp., London, UK
SOURCE: Carbohydrate Research (1969), 11(2), 287-8
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB 1,6-Anhydro-4-O-p-tolylsulfonyl-β-D-glucopyranose was boiled in (CH2OH)2 with KHF2 for 75 min to give 47% 1,6-anhydro-4-deoxy-4-fluoro-β-D-glucopyranose (I), m. 118-20° [α]D -53° (H2O), which after hydrolysis with M HCl gave 56% 4-deoxy-4-fluoro-D-qlucose, m. 187-9°, [α]D 26 → 49° (H2O), β-tetraacetate (II) m. 127-9°, [α]D -32° (CHCl3). The configuration of the products was established by 1H and 19F NMR spectroscopy on I and II.
IT 27108-04-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 27108-04-9 HCAPLUS
CN β-D-Glucopyranose, 4-deoxy-4-fluoro- (CA INDEX NAME)

Absolute stereochemistry.